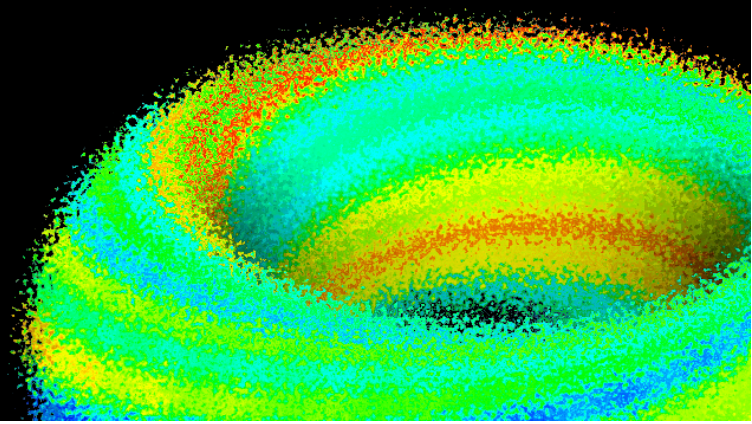
Supercomputing for Fusion Energy Applications

Fusion Group



Barcelona Supercomputing Center
Centro Nacional de Supercomputación

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February 18, 2016

Outline

Introduction to Plasma Physics

Supercomputing for Fusion Energy Applications

Particle-in-Cell Codes

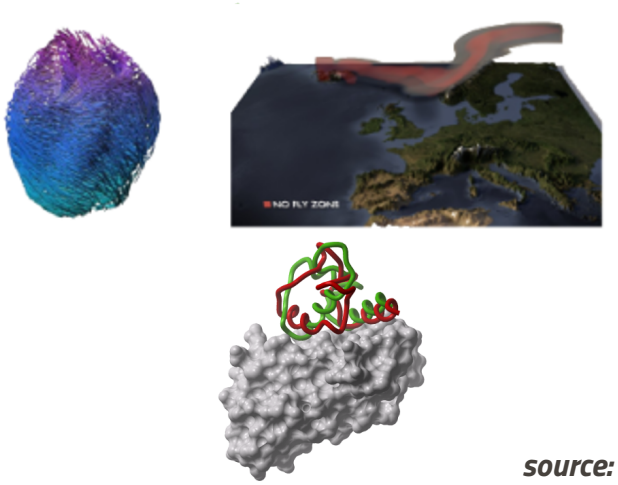
Fusion Group

Outline

- Introduction to Fusion Energy
- Supercomputing for Fusion Energy Applications
- Particle-in-Cell Codes
- Fusion Group

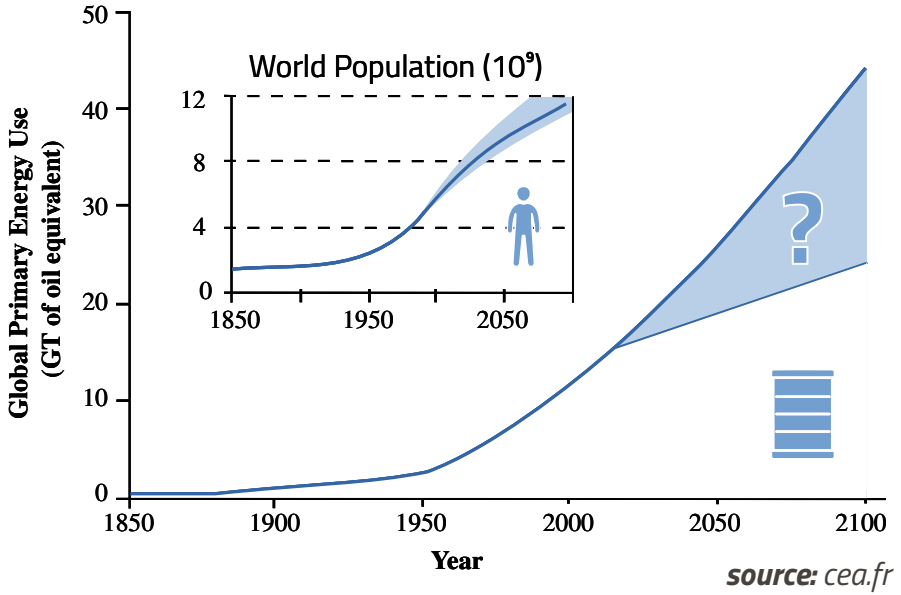
Motivation

- Grand scientific challenges are the driving force for High Performance Computing (HPC) evolution

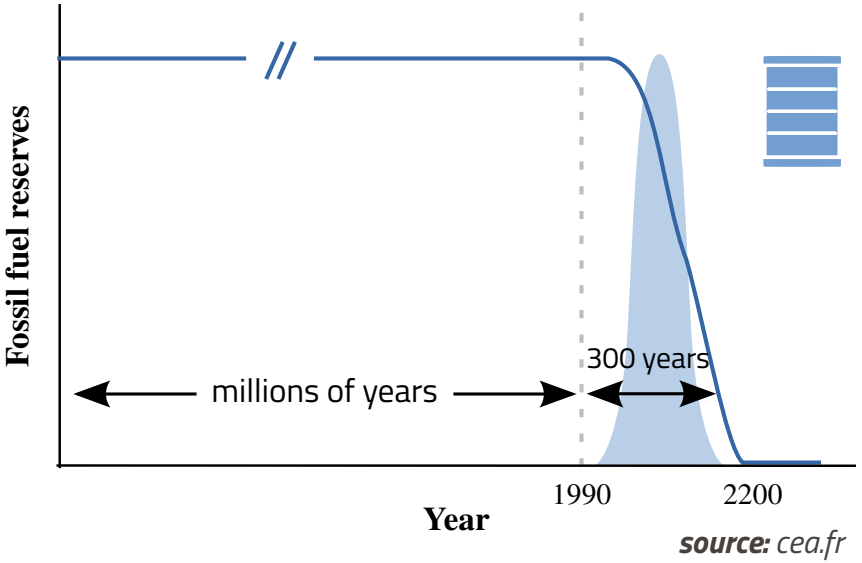


source: bsc.es

- Future energy needs



source: cea.fr



source: cea.fr

Objective

It is considered a key sector, e.g.

EUROfusion, EUFORIA...

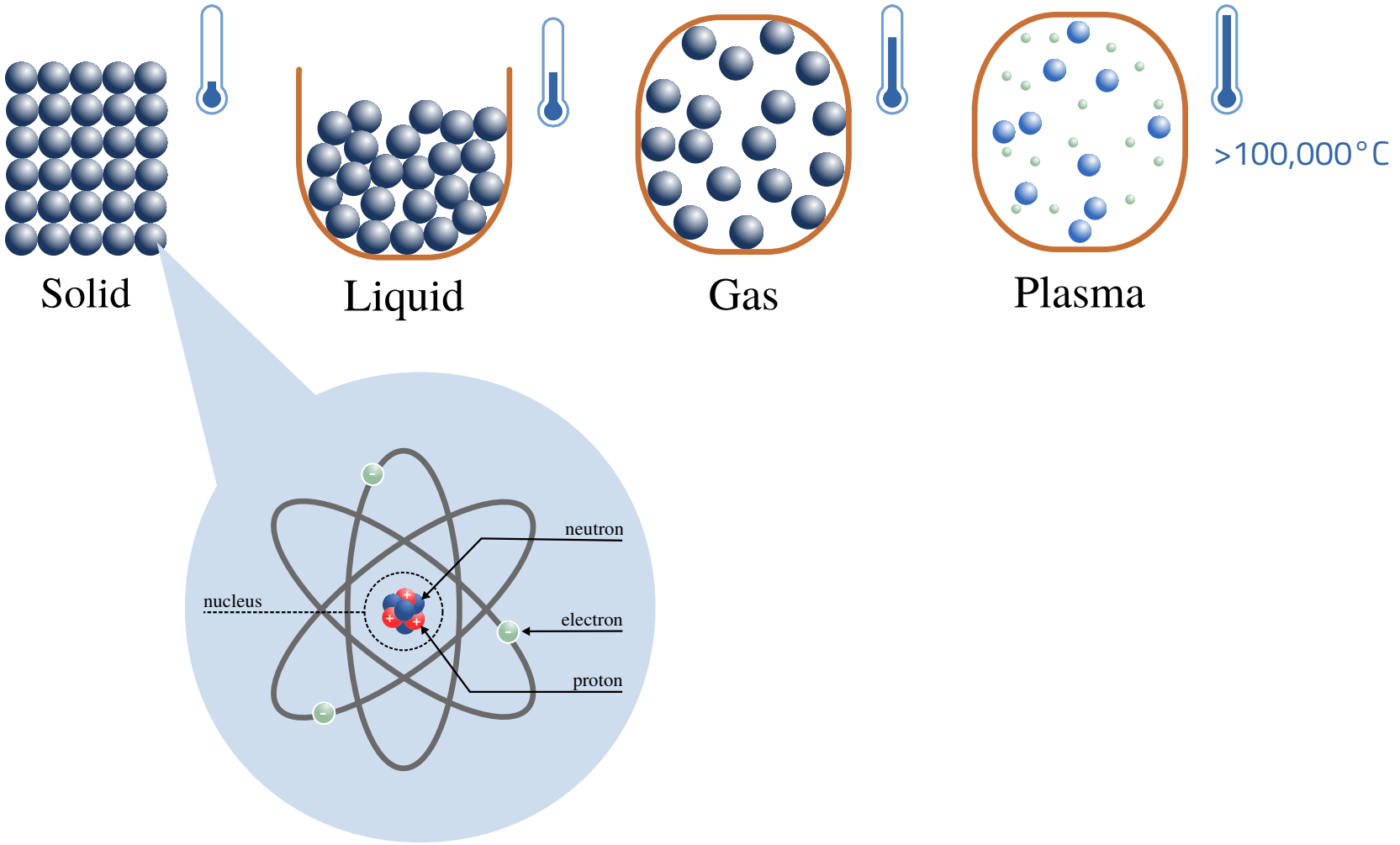
Context

- Plasma physics (from 1950's)
  - experiments are difficult and expensive (e.g. fusion reactors) → computational simulations
  - $\geq 10^{20}$ particles / m^3 (tokamak) → require intensive computation
- Plasma codes
  - codes suffer from the defects of dealing with idealized configurations due to lack of computing power → process level parallelism
  - for new fusion reactors (ITER) → more physics and detail → need to adapt to new platforms

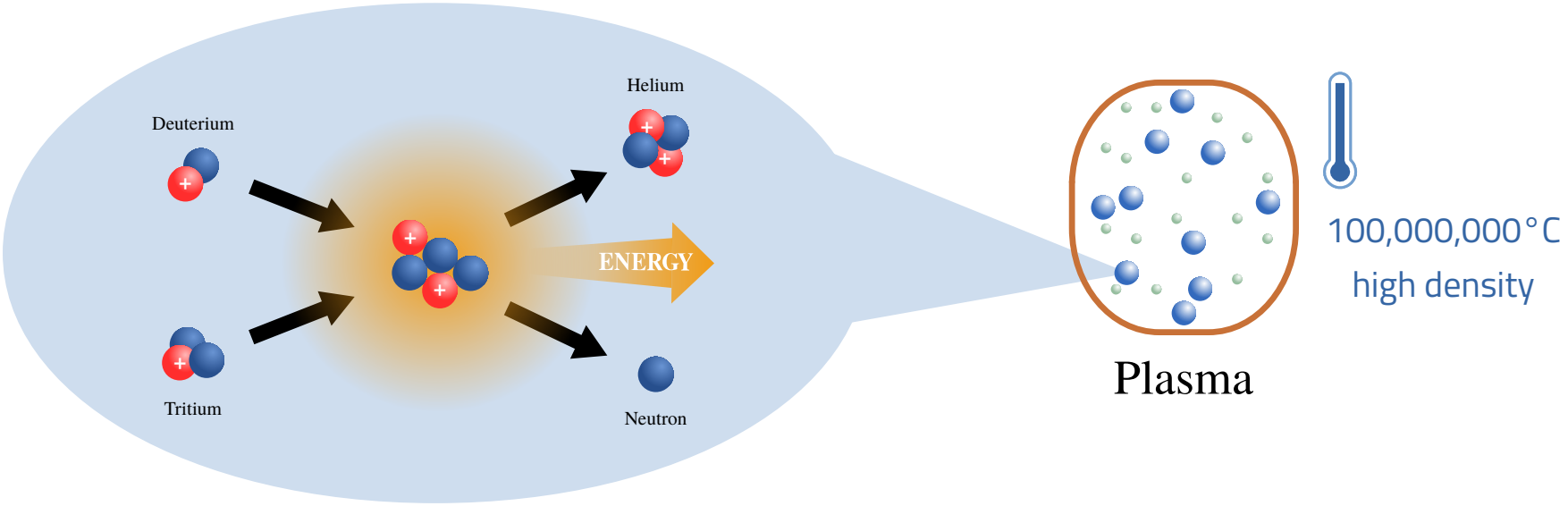
Context

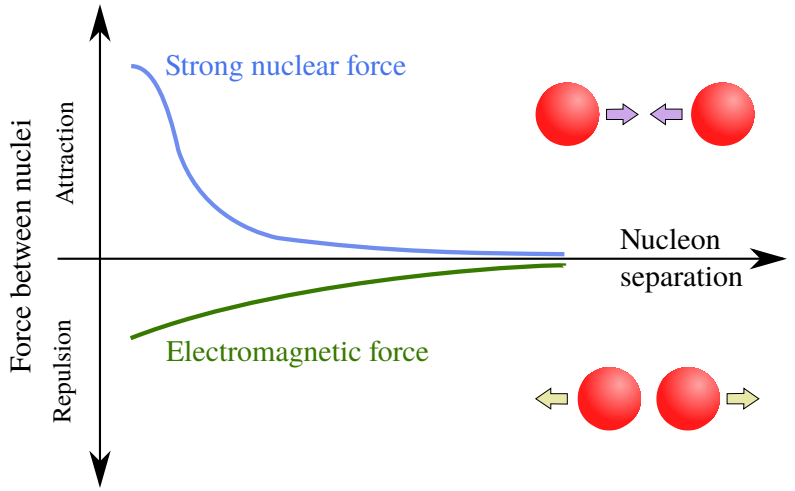
- High-Performance Computing (HPC) has evolved from single-core architectures
  - power efficiency has become a primary concern
    - multi-core architectures
    - Mont-blanc project → mobile processors
- If we want to add more physics and detail → we need to adapt plasma codes to new platforms

- What is Plasma?



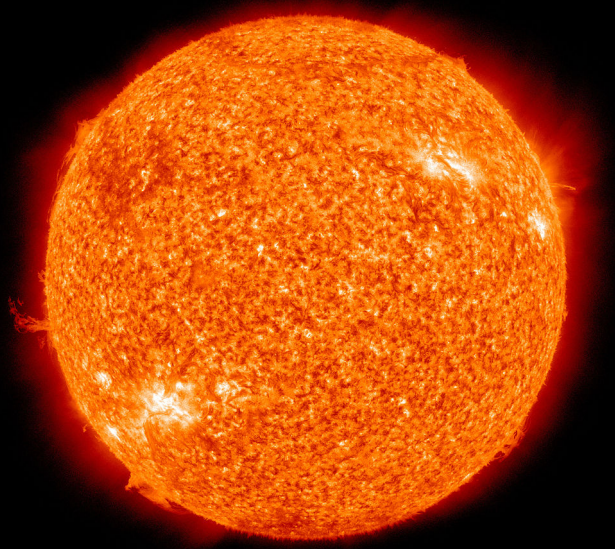
- What is Nuclear Fusion ?





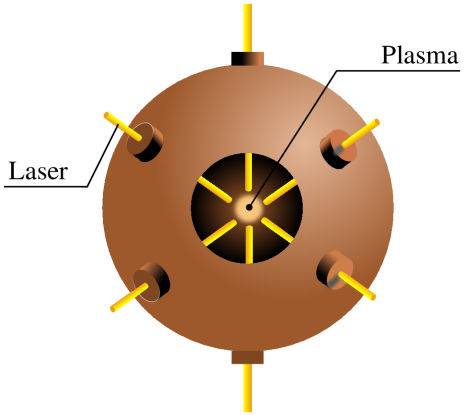
- Fusion Reactors (Space)
  - Gravitational confinement

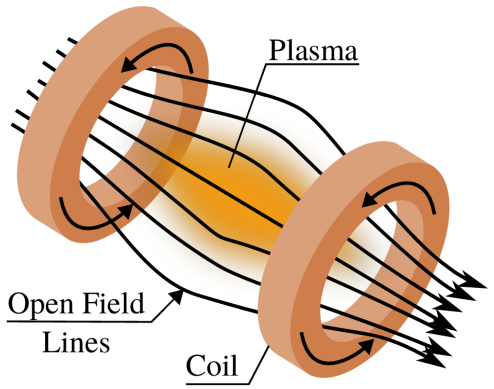
To confine the plasma to create the conditions necessary for fusion reactions to occur



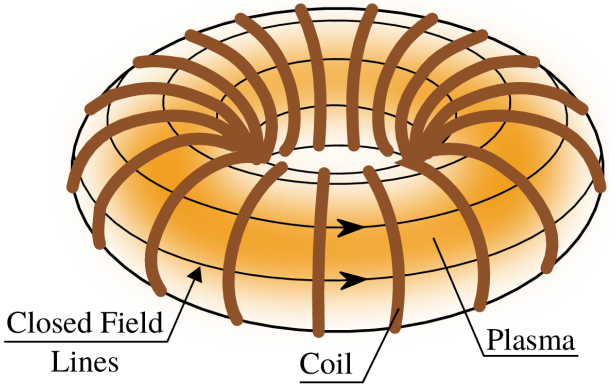
source: *nasa.gov*

- Fusion Reactors (Earth)
  - Inertial confinement
  - Magnetic confinement

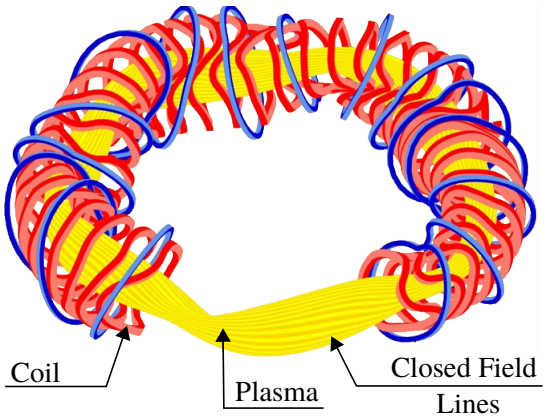




Magnetic Mirrors

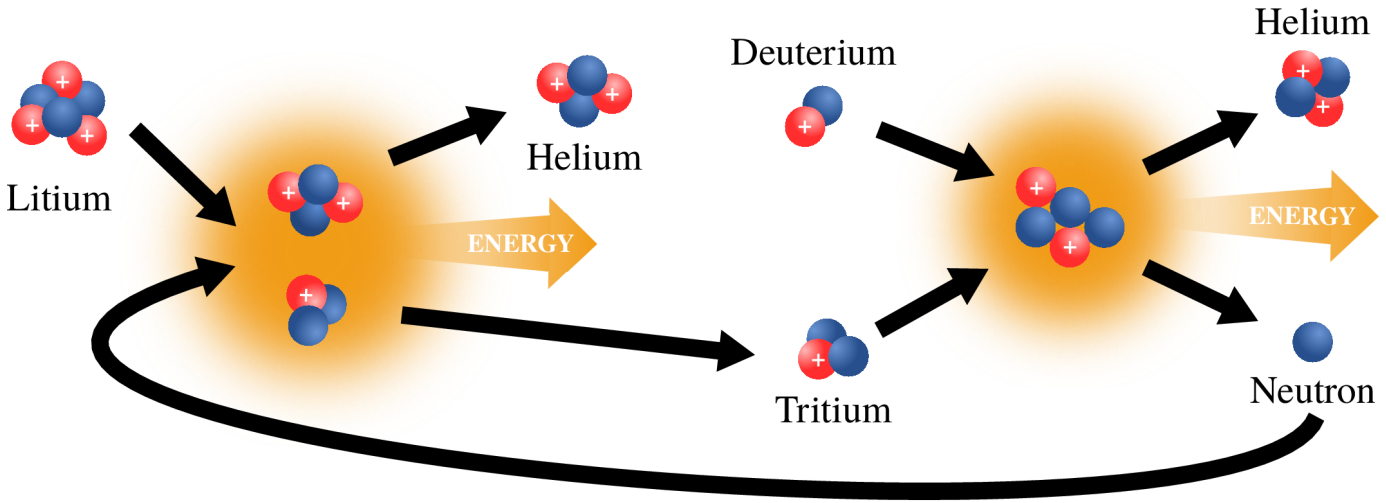


Tokamak



Stellarator

- Fusion Reaction
  - Deuterium-Tritium Fusion

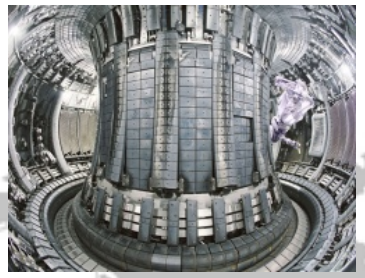


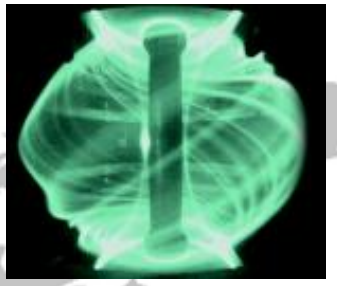
$$\mathrm{Li}^6 + n \rightarrow T + He^4 + 4.8MeV$$

$$\mathrm{D{+}T} \rightarrow He^4(3.5MeV) + n(14.1MeV)$$

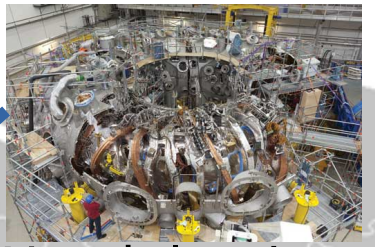
Fusion Reactors

- Fusion reactors in the world



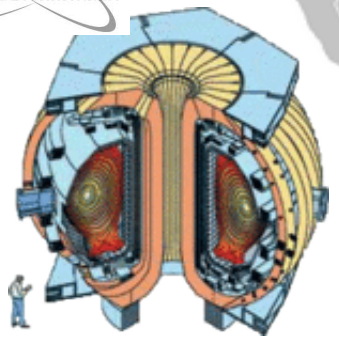


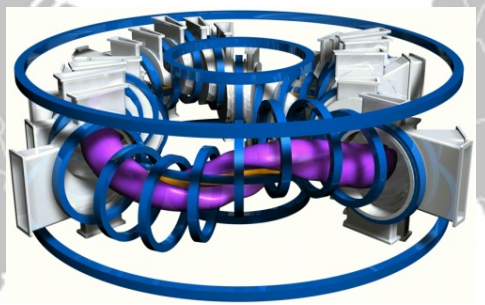
JET (EU) and MAST (UK)



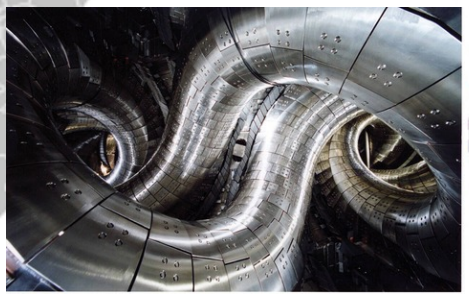
Wendelstein 7-X (Germany)

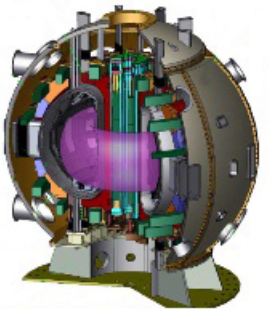
DIII-D NATIONAL FUSION FACILITY





TJ-II (Spain)

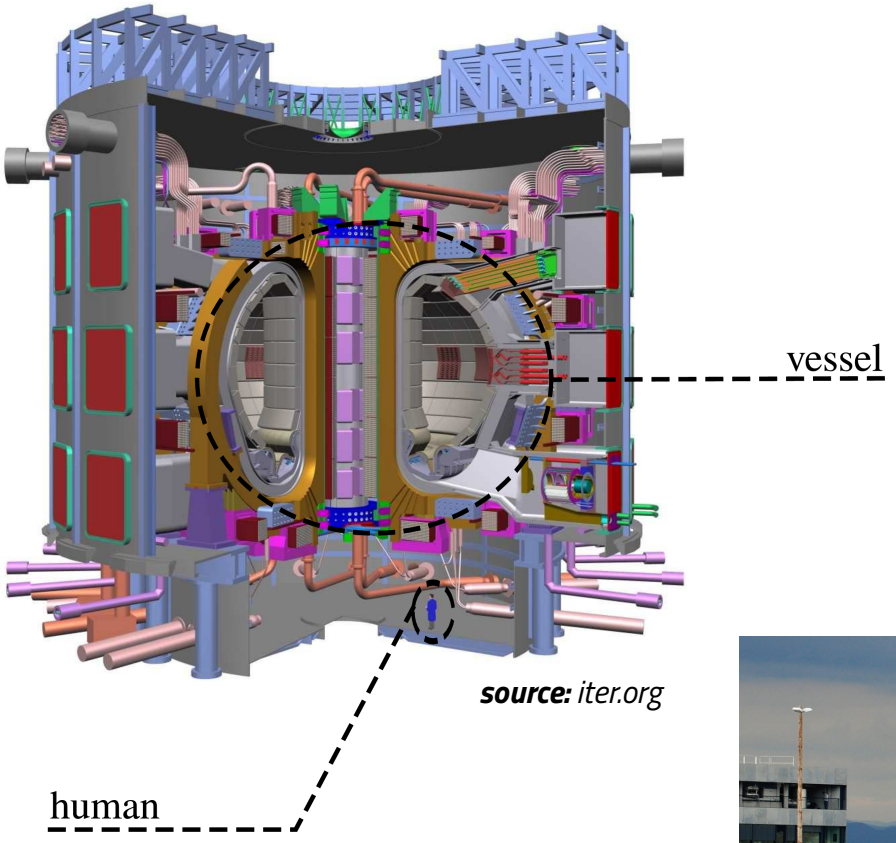




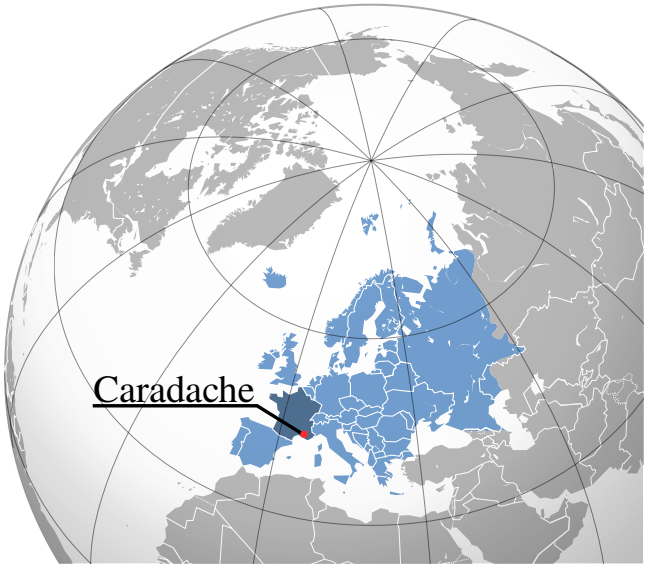
LHD and JT60U (Japan)

Fusion Reactors

- ITER *"The way"*



source: *iter.org*



source: *iter.org*

Fusion Reactors

- ITER *"The way"*

source: *The Daily Conversation*

- Maxwell's equations

Gauss's law
$$\nabla \cdot \vec{E} = \frac{1}{\varepsilon_0} \sum_{\alpha} q_\alpha \int f_\alpha d^3 v$$

Gauss's law for magnetism
$$\nabla \cdot \vec{B} = 0$$

Faraday's law
$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

Ampère's law
$$\nabla \times \vec{B} = \mu_0 \sum_{\alpha} q_\alpha \int \vec{v} f_\alpha d^3 v + \frac{1}{c^2} \frac{\partial \vec{E}}{\partial t}$$

- Poisson's equation

$$\nabla^2 \phi = -\frac{q}{\varepsilon_0} \int f\left(\vec{x}, \vec{v}, t\right) d\vec{v}$$

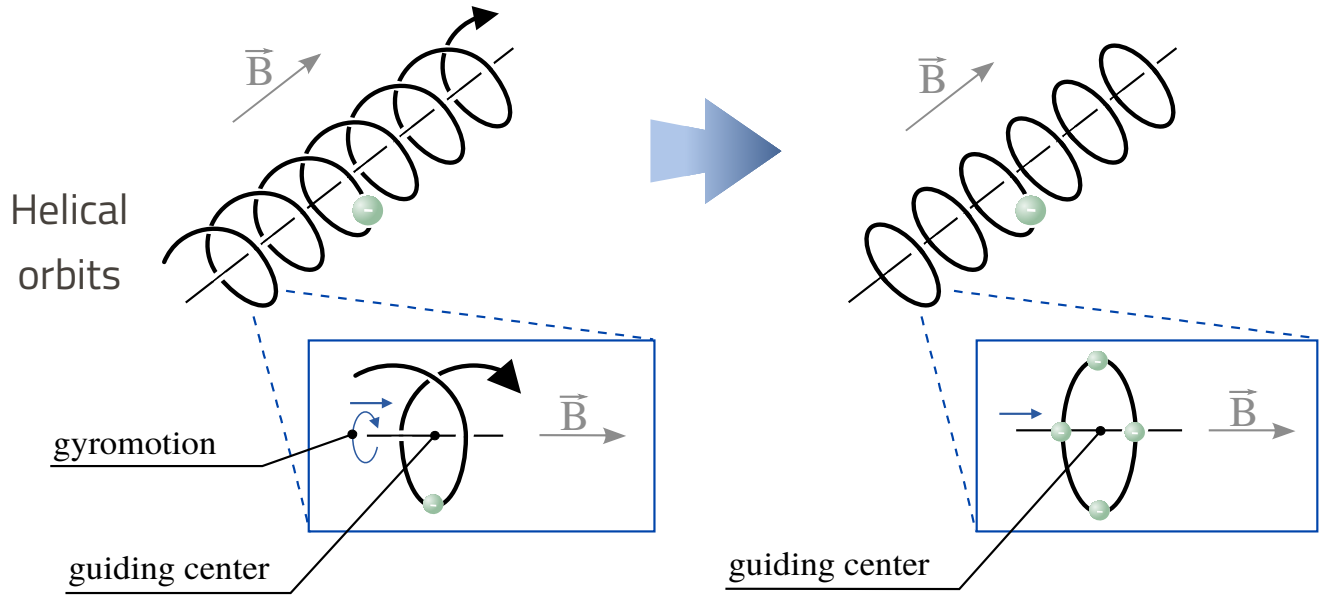
Plasma Physics

- Transport equation (6d+t)

$$\frac{\partial f_\alpha}{\partial t} + \vec{v} \cdot \frac{\partial f_\alpha}{\partial \vec{x}} + \frac{\vec{F}^{tot}}{m_\alpha} \cdot \frac{\partial f_\alpha}{\partial \vec{v}} = C_\alpha$$

collision-less
$C_\alpha \approx 0$

- Gyrokinetic approximation

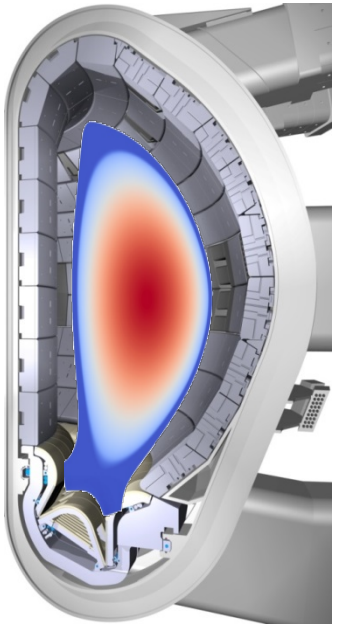


(5d+t)

Outline

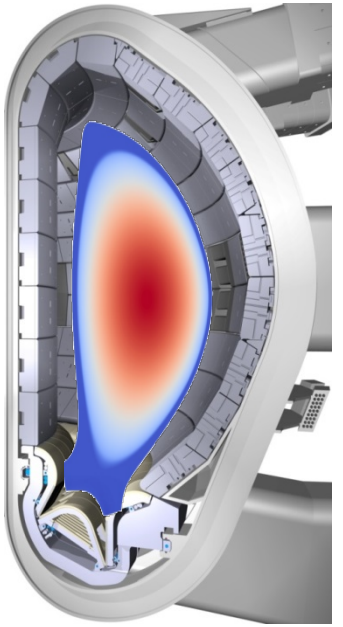
Big Questions

- How do we produce stable plasmas?
  - Can we feedback control it?
  - How do we sustain a fusion plasma in close proximity to a vacuum vessel?
- How do the particles and heat leak out?
  - How do we minimize the losses?
- How can turbulence finish confinement?
  - Could we trigger turbulence reduction externally?



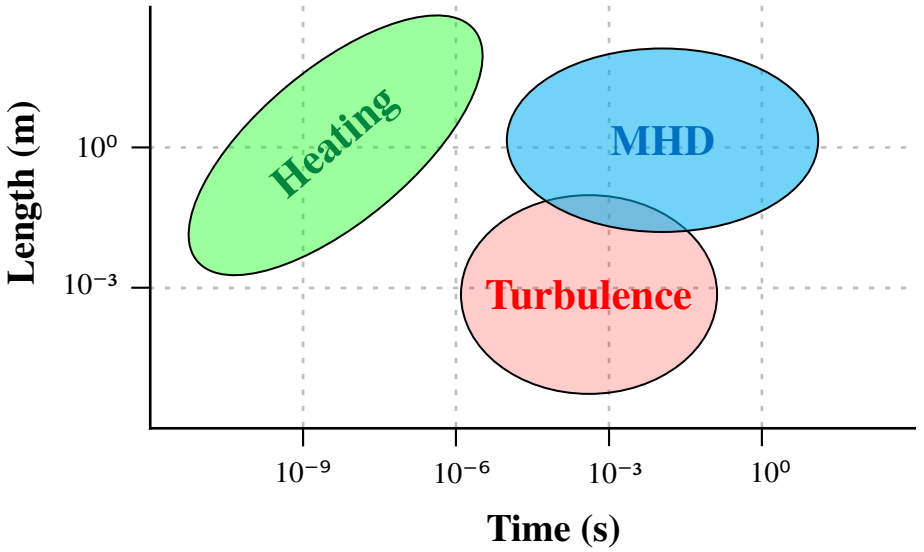
Big Questions

- We need fusion modelling to understand and control the plasma dynamics in tokamak and the implications for ITER:
  - Which materials do we use in fusion reactor?
  - How could we handle the intense flux of power, neutrons and charged particles on the wall?



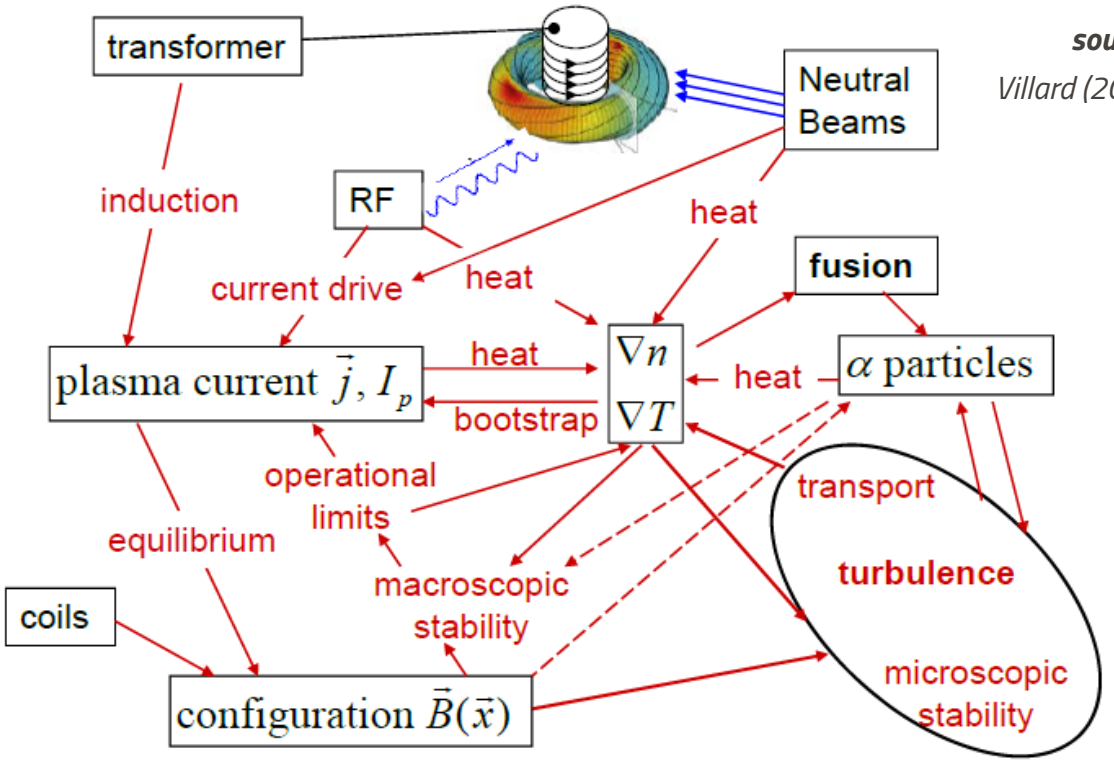
Fusion Modelling

- There are many non-linear phenomena in fusion plasmas
  - Energetic ions
  - Core transport
  - Transport Barrier
  - Non-inductive CD
  - RF Heating
  - NBI Heating
  - Neutral Transport
  - MHD stability
  - Impurity Transport
  - Turbulent Transport
  - Plasma Wall Int.
  - Divertor Plasma
  - SOL Transport
  - and more …
- Wide ranges of time scale and spatial scale interact each other.
  - Time scale: 10^{-12} s ~ 1000s
  - Spatial scale: 10um ~ 10m



Fusion Modelling

- Unfortunately, these phenomena can not be modelled in a single simulation in a reasonable time.



source: *Villard (2010)*

- Therefore, supercomputing is needed to simulate
  - Integrating relevant phenomena combining modelling codes in a consistent manner
  - Dealing with various levels of physics model

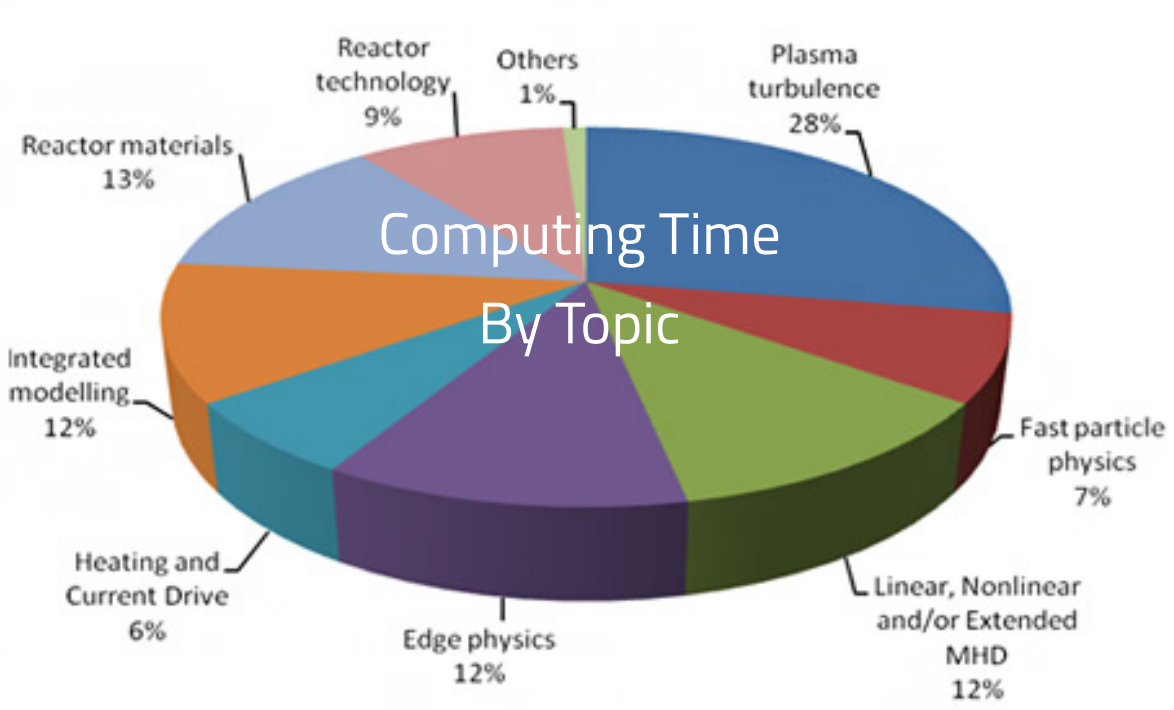
Supercomputing

- To sum up, it allow us to face these problems:
  - to analyze experimental data on fusion plasmas
  - to improve understanding of the physics involved and to validate the theoretical models and the modelling codes
  - to prepare scenarios for ITER operation
  - to predict the performance of the ITER facilities
  - ...

Supercomputing

- Example: **HELIOS** supercomputer
  - Located in Rokkasho (Japan)
  - Only for fusion simulation projects
  - 4410 bullx B510 compute nodes
  - Each node contains 2 Intel 8-core Sandy Bridge EP processors with 58 GB of RAM
  - 1.52 PFLOPS

The HELIOS Supercomputer system at IFERC-CSC.

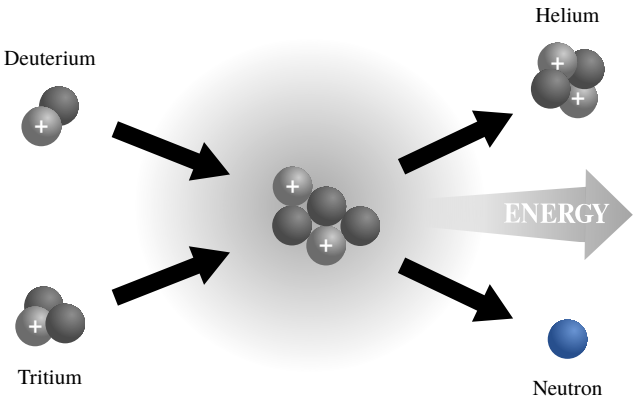


Modelling of Fusion Plasmas

- Fusion neutronics
- Fast particle physics
- MHD in fusion plasma
- Plasma turbulence

Modelling of Fusion Plasmas

- Fusion neutronics
  - Fusion plasma is a source of neutrons which impinge on all material surrounding the plasma.
  - Through interaction with neutrons, materials become activated and subsequently, emit decay photons.



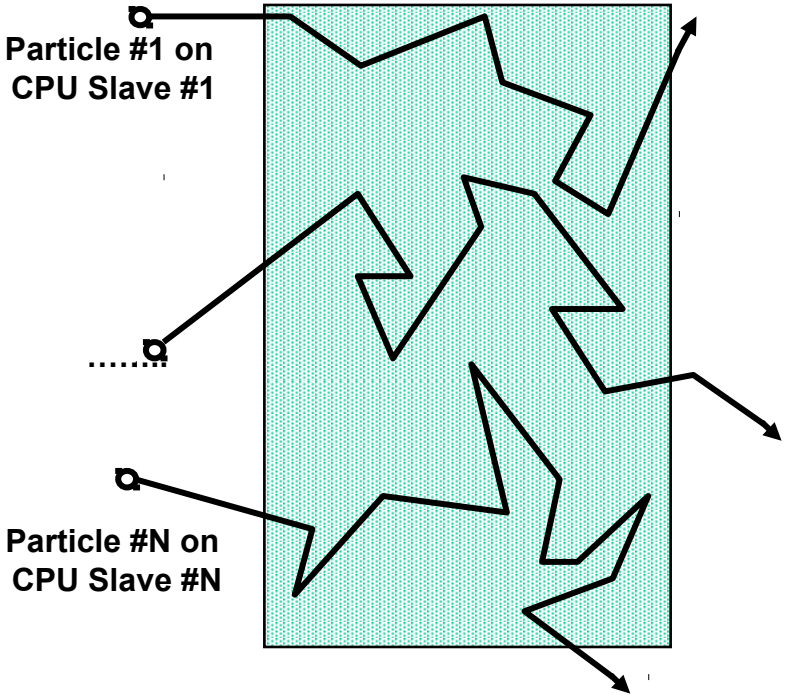
  - The resulting shut-down dose rate is an occupational health issue.

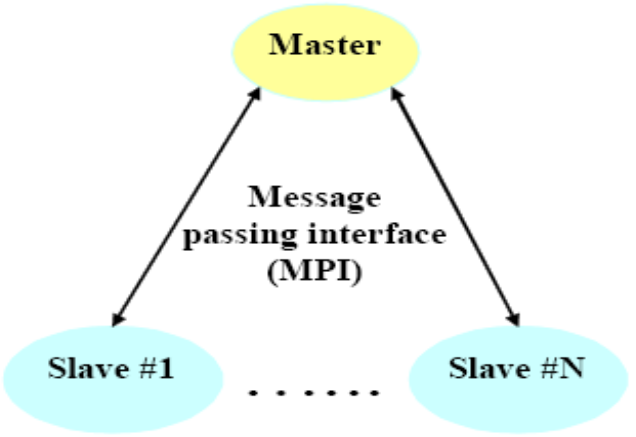
Two families of neutronics codes:

- **Deterministic**: PARTISN, DOORS, DEVONO, ATTILA,..
- **Monte Carlo**: MCNP, TRIPOLI,...

Modelling of Fusion Plasmas

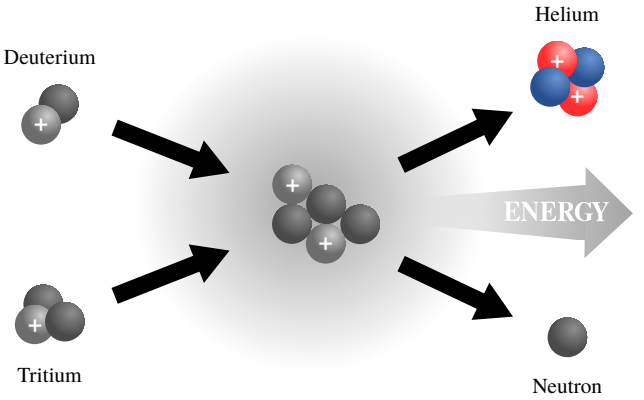
- Fusion neutronics
  - Monte Carlo codes
  - Tracking of individual particle pathways on microscopic level in complex 3D geometries of fusion devices





Productive parallel run on
slave processors

- Fast particle Physics
  - Different types of 'fast' particles (non-thermal) exist in a fusion reactor:
    - Helium-4 ions, neutral beam injected ions, particles heated by RF waves, ...



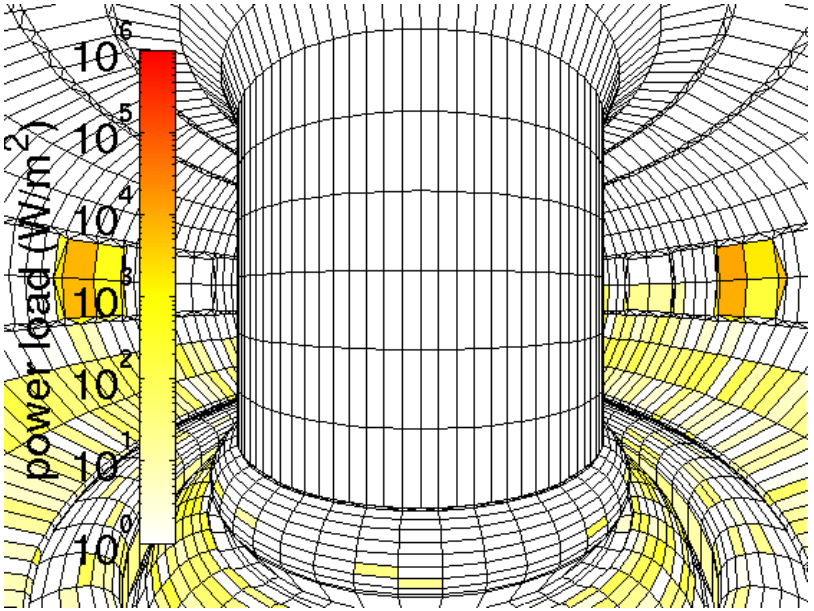
  - These particles will collide with other plasma particles. It can drive instabilities and possibly losses of fast particles can damage the surrounding materials and need to be kept at a tolerable level.

There are many codes:

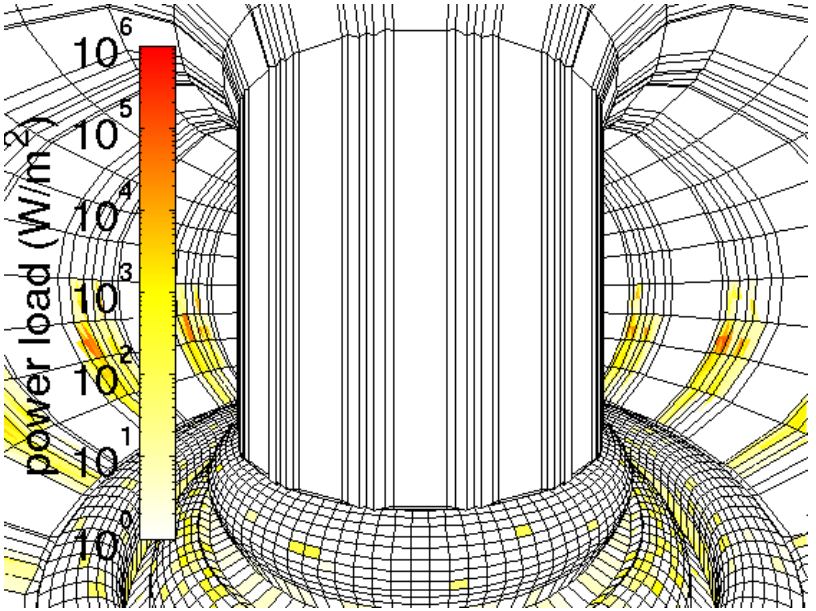
- OFMC-3D (Japan);
- SPIRAL (USA);
- DRIFT (Russia);
- ASCOT (Finland)...

Modelling of Fusion Plasmas

- Fast particle Physics
  - ASCOT: Racetrack for tokamak particles



Original wall w/ 2 limiters



Present wall design w/ poloidally extended 'continuous' limiters

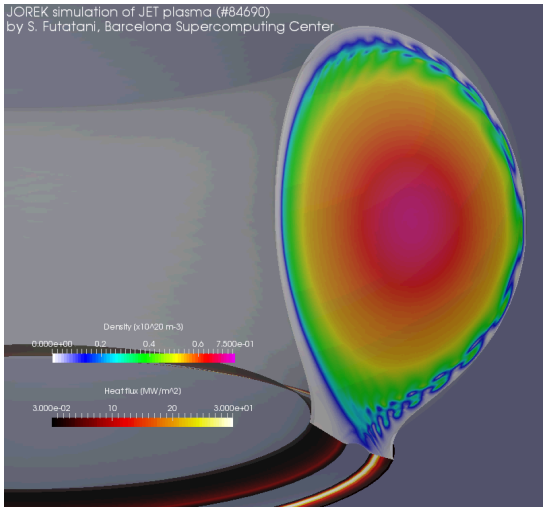
source: *Kurki-Suonio et al.*

Modelling of Fusion Plasmas

- Edge Localized Modes (ELMs)
  - A disruptive instability occurring in the edge region of a tokamak plasma
  - These instabilities can damage wall components, particularly divertor plates, due to their extremely high energy transfer rate
  - Safe ELMs for divertor:

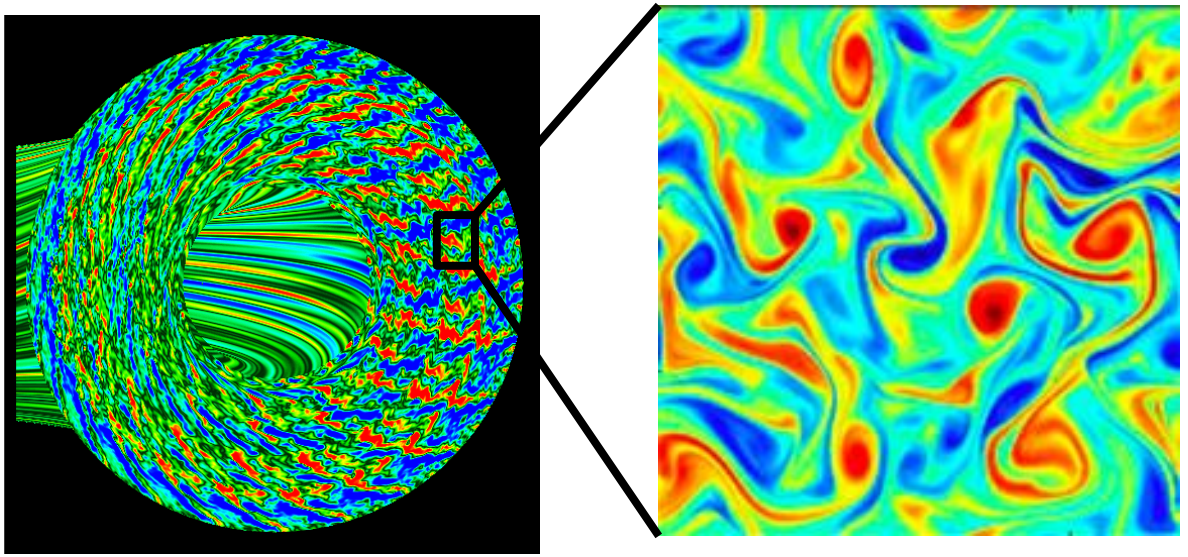
    $W_{ELM} < 1MJ$
  - Predictions for ITER:

    $W_{ELM} \sim 20MJ$



Modelling of Fusion Plasmas

- Plasma turbulence
  - Turbulence governs fusion plasma performance
  - Limits the maximum reachable density and temperature
  - Degrade the confinement



[Numerical Tokamak, Dorland et al.]

[Futatani et al.]

Outline

Introduction to Plasma Physics

Supercomputing for Fusion Energy Applications

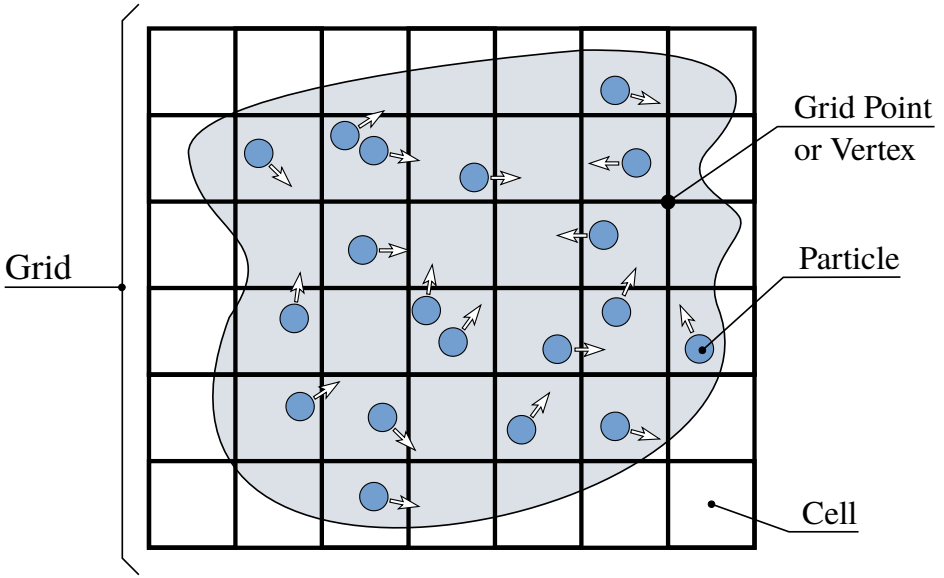
- Particle-in-Cell Codes

Fusion Group

Particle in Cell

- Particle-in-Cell (PIC) is a method to model physical systems whose behaviour varies on a large range of spatial scales.

- Two problems (trade-off) :
  - Macroscopic level, the dynamics is described by a continuum model
  - Microscopic level is modeled by a collection of discrete particles



Particle in Cell

- Algorithm

Initialize *particle* data

Initialize *grid* (field) data

while $t < t_{max}$ **do**

Compute particle contributions to the *grid*

Calculate the fields

Update forces on *particle* positions

Move *particles* to new positions

if display **then**

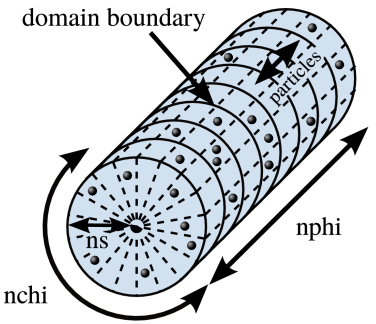
Print *particles* and *grid* data

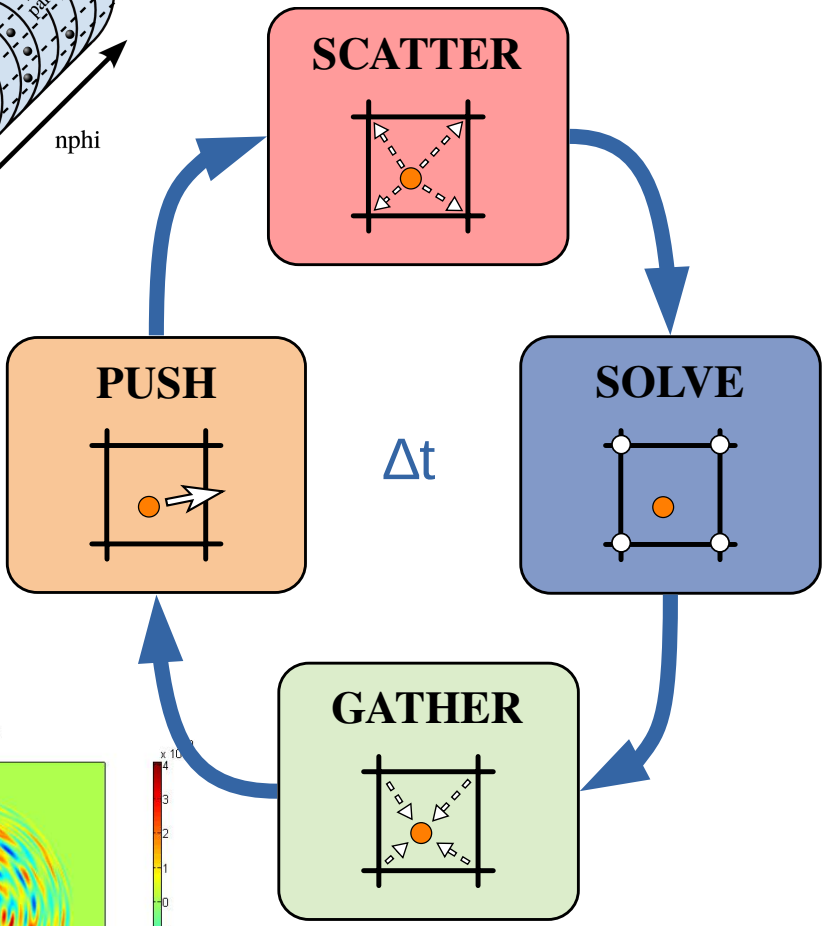
Print statistics

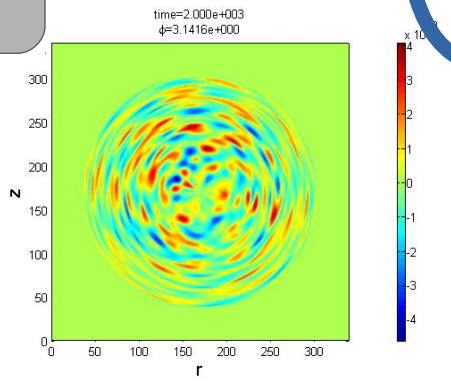
end if

$t \leftarrow t + t_{step}$

end while

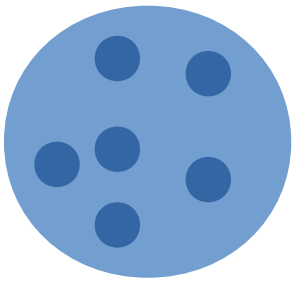


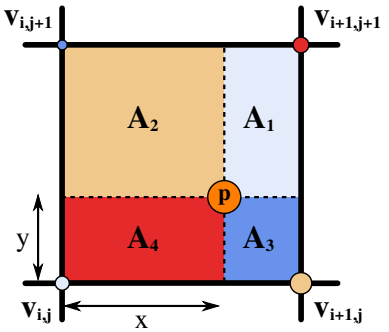


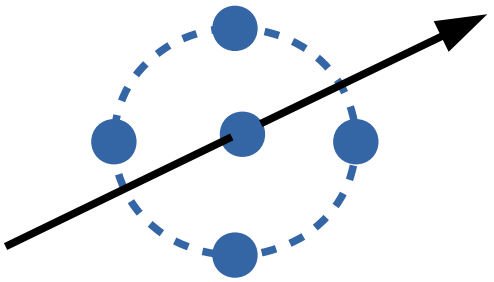


Particle in Cell

- PIC codes are very demanding in computational power
- Simplifications are introduced
  - Markers = *cloud of particles*
  - Linear interpolations (scatter and gather phases)
  - Collision-less
  - Gyrokinetic approximation: (6d+t) → (5d+t)



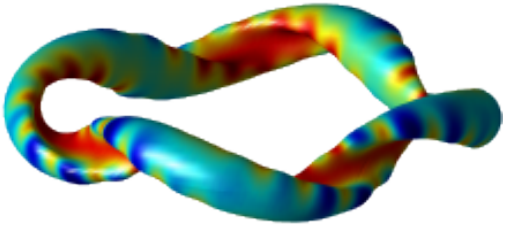




Particle in Cell

- Examples of Codes:
  - GENE
  - ELMFIRE
  - BIT1
  - EUTERPE
  - ...

- Gyrokinetic PIC code for the simulation of plasma microturbulence in 3D geometries (stellarators, tokamaks, etc)



source: *ciemat.es*

- Developers:

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

IPP Max-Planck-Institut für Plasmaphysik

- Collaborators:

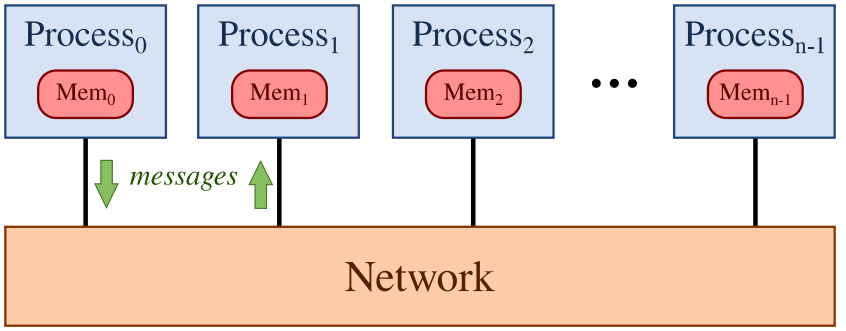
GOBIERNO DE ESPAÑA MINISTERIO DE CIENCIA E INNOVACIÓN

Ciemat Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas

BSC Barcelona Supercomputing Center Centro Nacional de Supercomputación

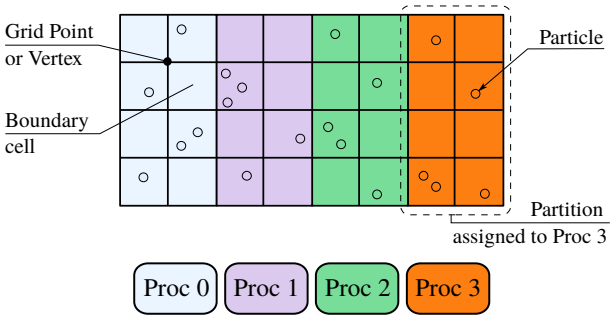
Particle in Cell

- Why to study them?
  - PIC is one of the most used methods in plasma physic simulations
  - PIC codes suffer from the defects of dealing with idealized configurations due to lack of computing power → process level parallelism
  - for new fusion reactors (ITER) → more physics and detail → need to adapt to new platforms
- Process Level Parallelism
  - Message Passing Model
  - Data decomposition can worsen the code performance



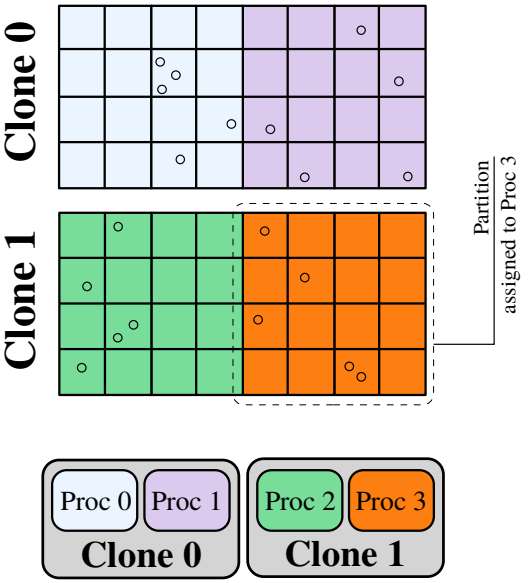
Process Level Parallelism

Domain Decomposition



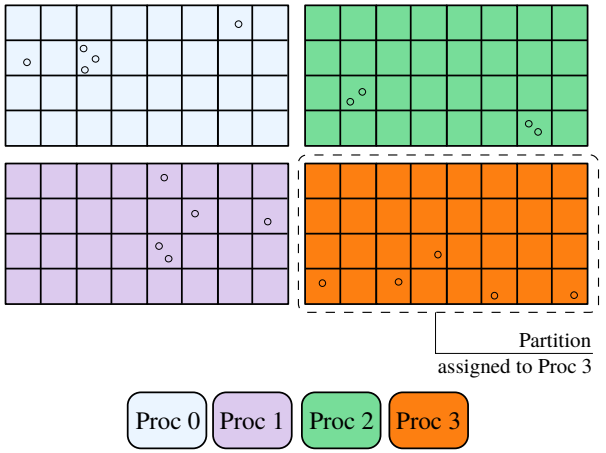
- ✔ Data locality
- ✖ Parallelization limited
- ✖ Unbalanced

Domain Cloning



- ✔ Scalability decoupled grid resolution
- ✔ Partial grid copy
- ✖ All-reduce communications

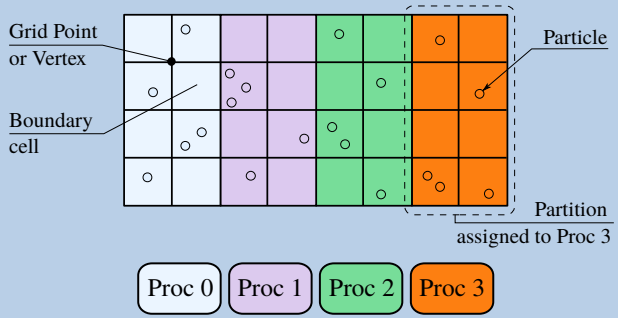
Particle Decomposition



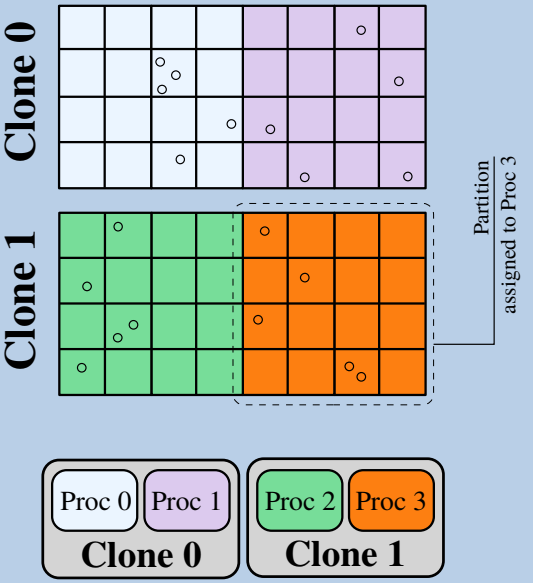
- ✔ Load balanced
- ✖ Expensive all-reduce
- ✖ Whole grid copy
- ✖ Not suitable for HPC

Process Level Parallelism

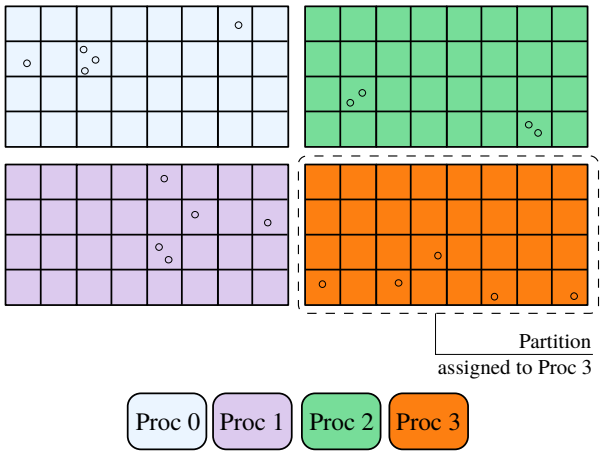
- Domain Decomposition



- Domain Cloning



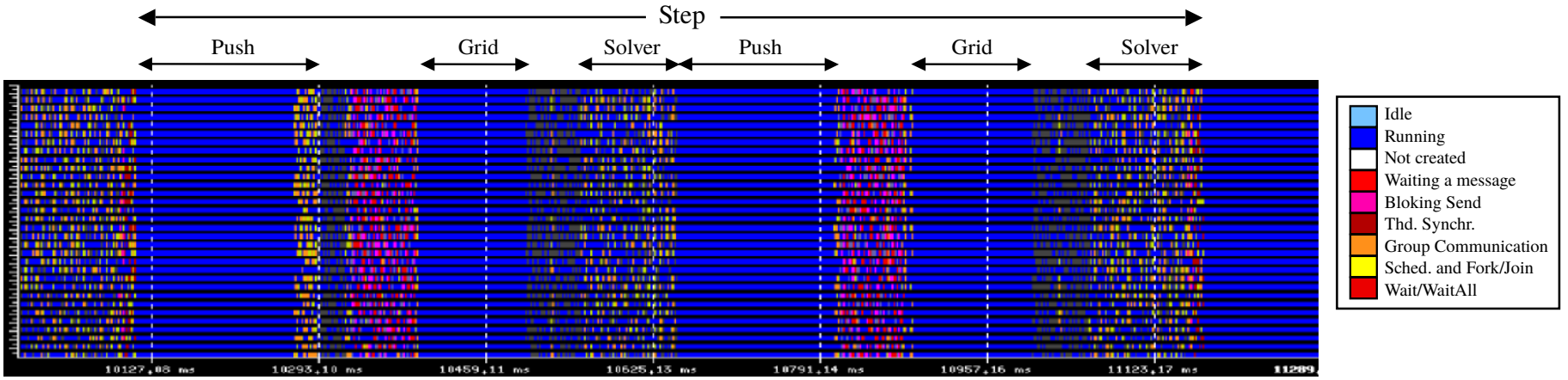
- Particle Decomposition



EUTERPE

Process Level Parallelism

- Load Balancing

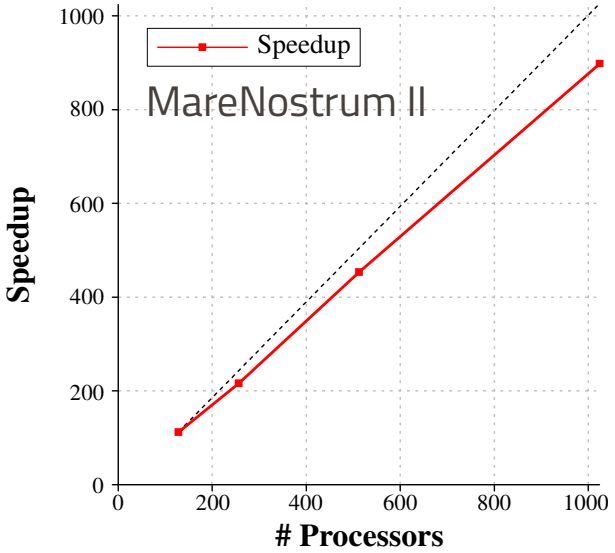


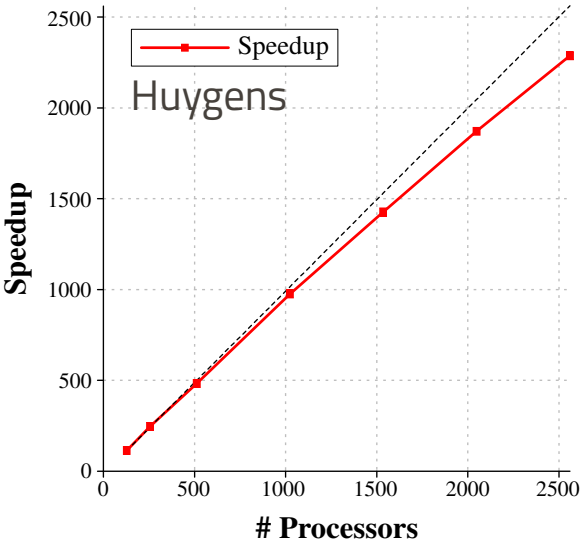
Domain Decomposition

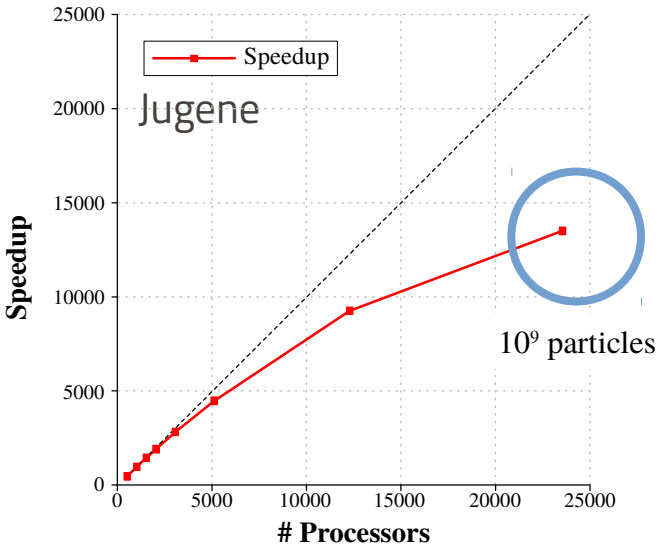
MareNostrum II

Process Level Parallelism

- Strong Scaling

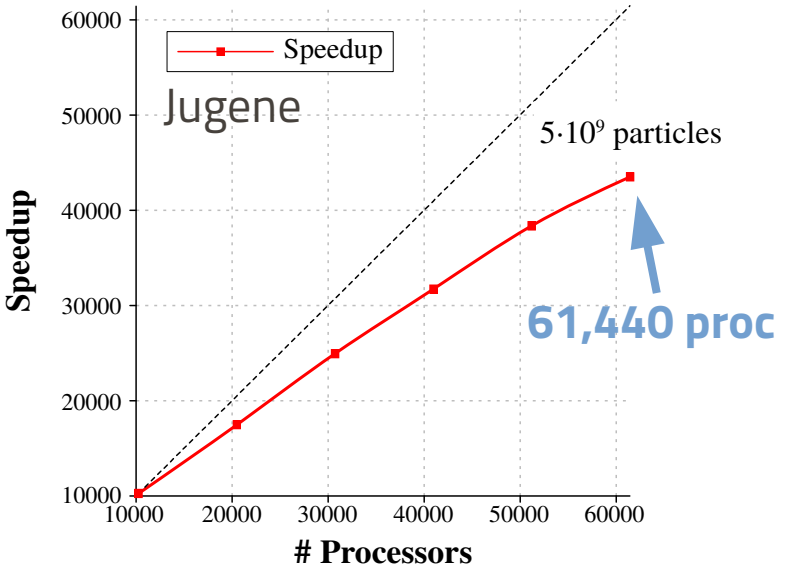






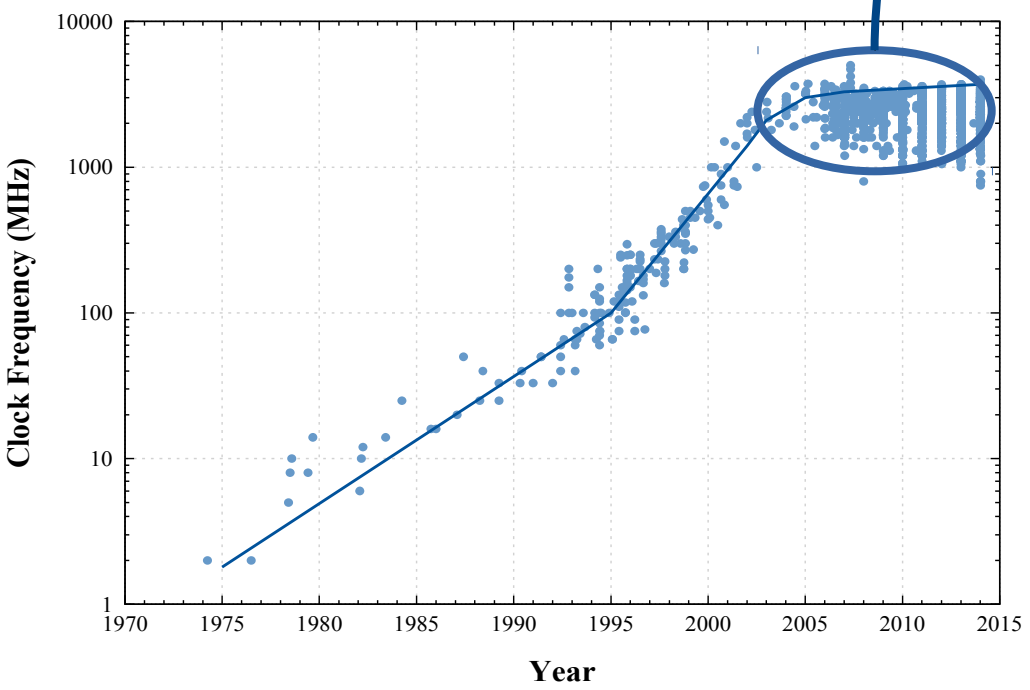
$$S(n) = \frac{T(1)}{T(n)}$$

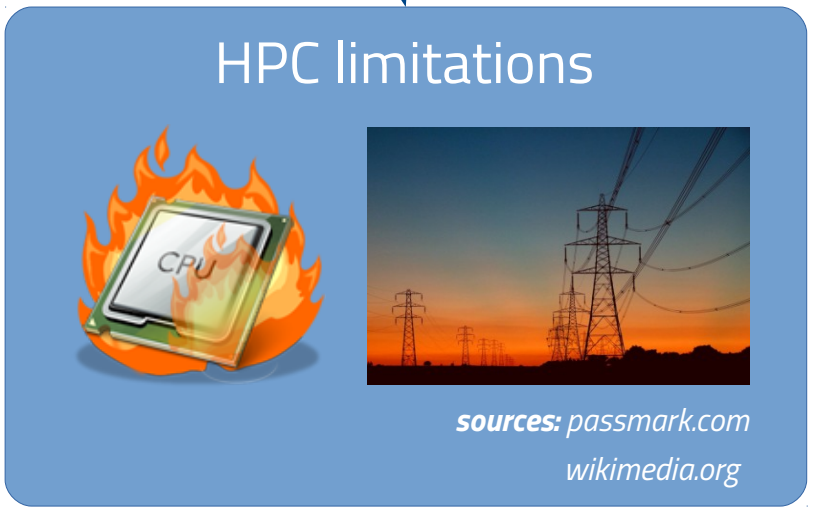
Domain Cloning

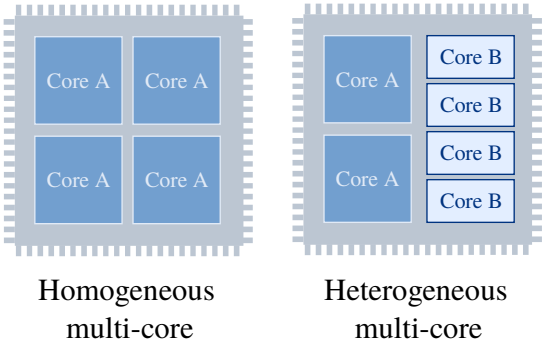


Multi-core Parallelism

- Evolution







Homogeneous multi-core

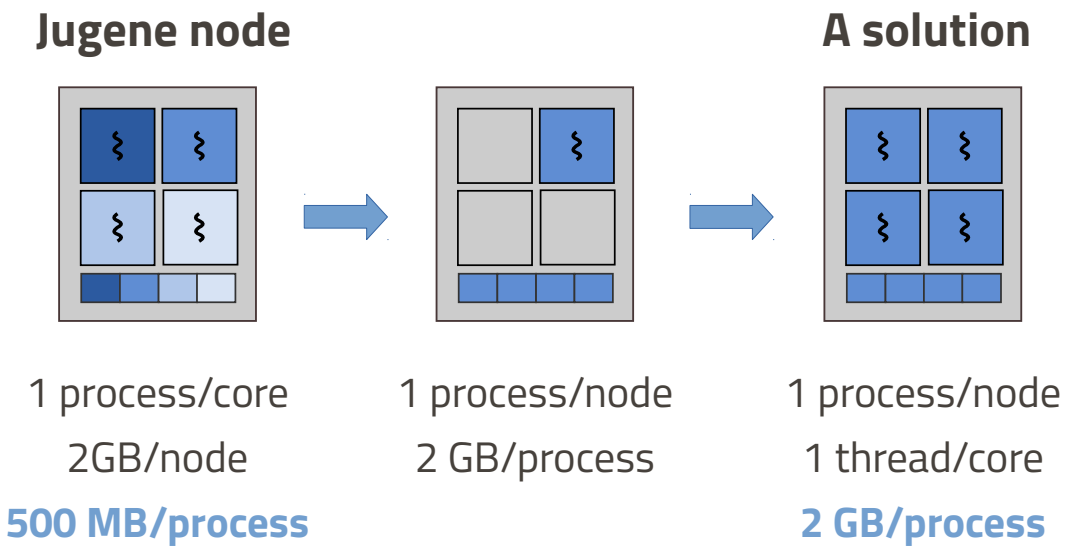
Heterogeneous multi-core

Multi-core Parallelism

- Influence on the codes
  - ✖ Limited space!

    ↓

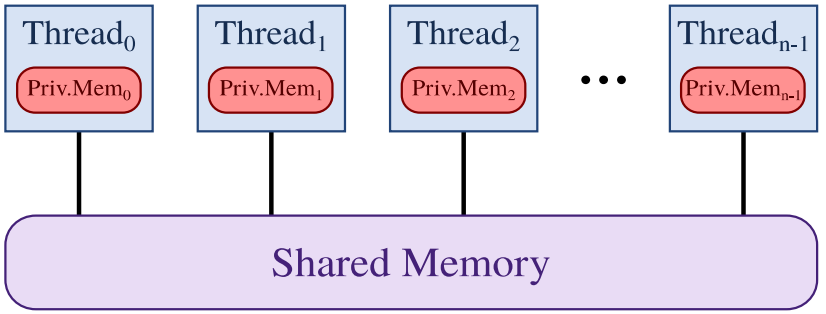
    Limited problems to solve or waste resources



- It is a need to adapt codes to new architectures to exploit all level of parallelism. Otherwise, we are paying for resources not used in HPC centers.

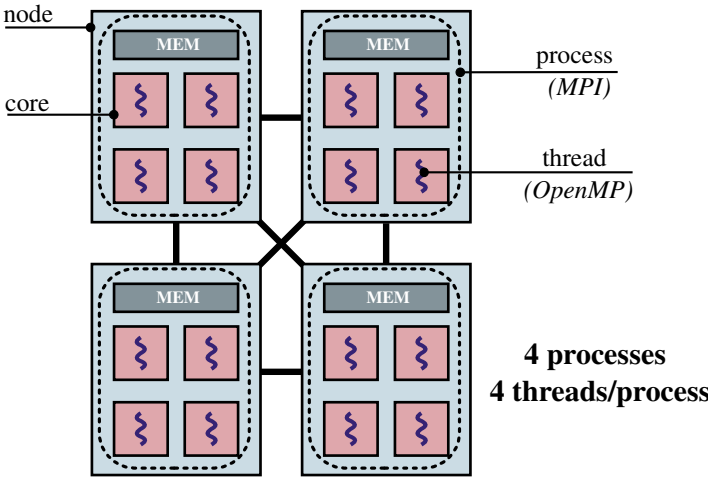
Thread Level Parallelism

- Shared Memory Model



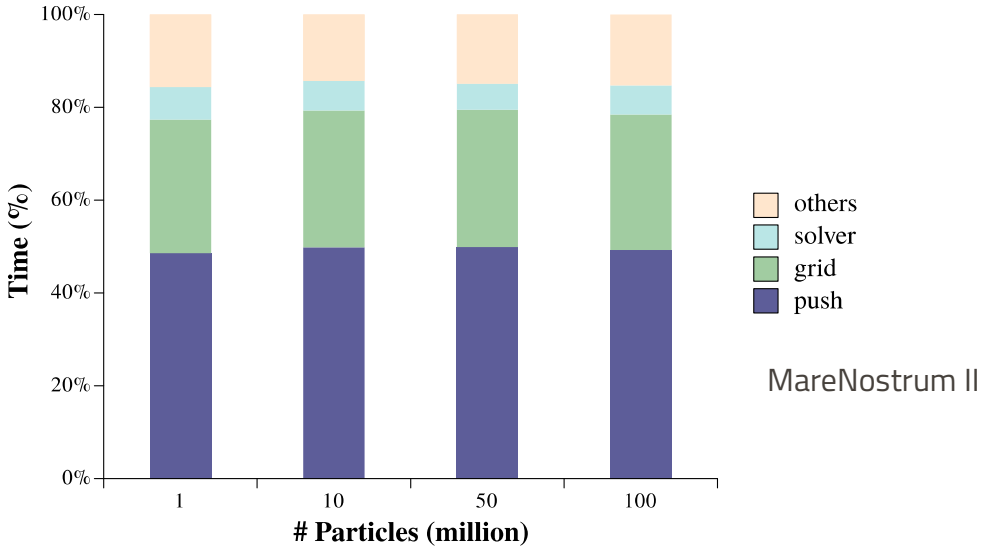
OpenMP

- Hybrid Version

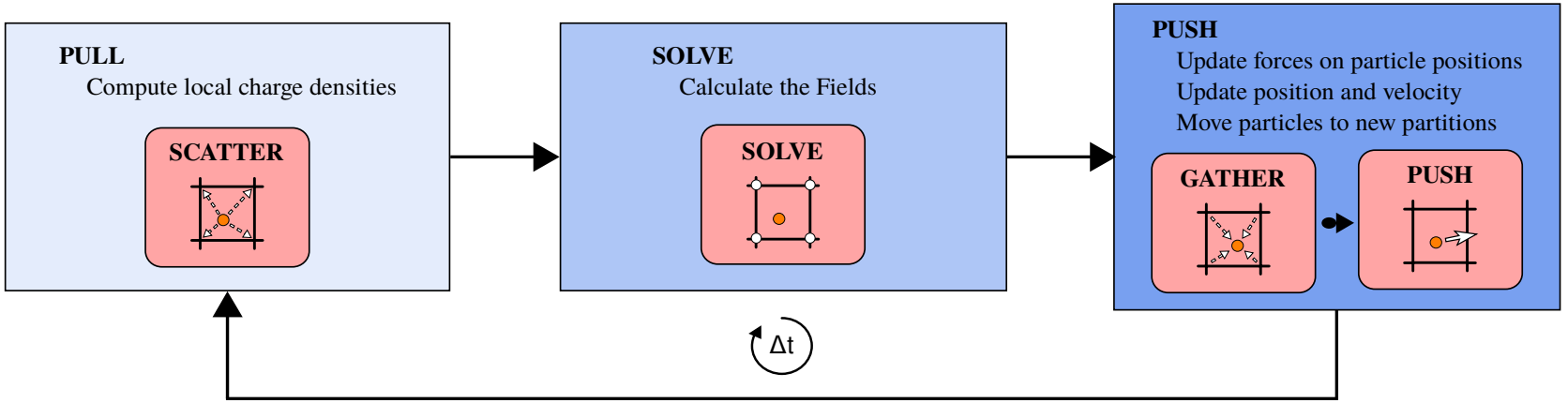


Thread Level Parallelism

- Time Distribution (EUTERPE)



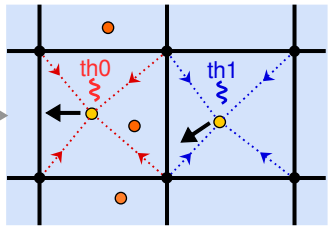
MareNostrum II

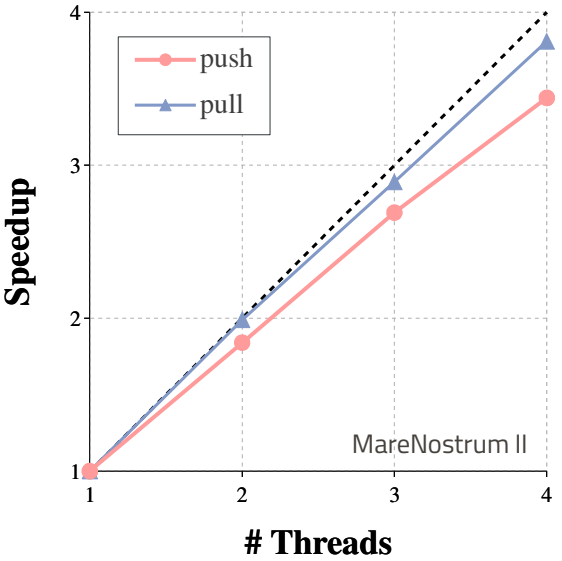


Thread Level Parallelism

- Push

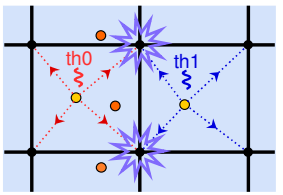
```
...
do ip = 1, npart_loc
   (rt,zt,phit) = pic_loc(ip)
   ...
   call getfield (rt,zt,phit...)
   ...
   if (diag_flag) then
      ...
   endif
enddo                          PARALLEL DO
...
```

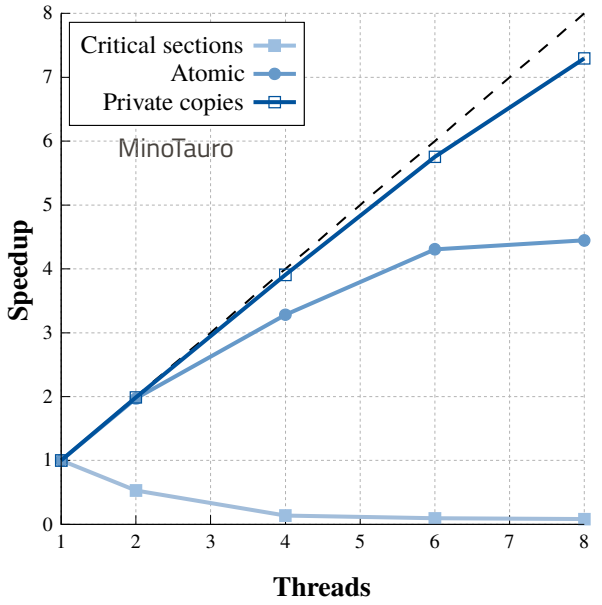




- Pull

```
rho = 0.0
...
do  ip = 1, npart_loc
   navg = gyroring_points(ip)
   ...
   do  l = 1, navg
      (s,chi,phi) = gridcell(ip,l)
      ...
      do  p = 1, 4
         (i,j,k) = gridvertex(s,chi,phi)
         rho(i,j,k) = rho(i,j,k) + ...
      enddo
   enddo
   ...
enddo                          PARALLEL DO
...
```





Thread Level Parallelism

- Pull Phase Code

```
numthrds = OMP_GET_MAX_THREADS()
ALLOCATE (rho_OMP(islw:isup, jclw:jcup, kplw:kpup, numthrds))
rho_OMP(:,:,:,:) = 0.0
rho(:,:,:) = 0.0
...
!$OMP PARALLEL DO                                                    &
!$OMP SCHEDULE (STATIC)                                              &
!$OMP DEFAULT  (NONE)                                                &
!$OMP PRIVATE  (ip, rt, zt, phit, vpart, wt, mut0, cosalp, pvol, s_gc,    &
!$OMP           chi_gc, b_abs, vperp2, u_bulk, ze_maxw, ztval_inv,        &
!$OMP           zvth2_inv, zf0, zphi_adi_val, za_par_adi_val, rhog, navg, &
!$OMP           wght, wght_cur, zcos1, zsin1, l, rt_x, zt_x, st_x,        &
!$OMP           chit_x, k, k_loc, wphi, phase, i, ws, j, wchi, kc, kkc,   &
!$OMP           temp1, jc, jjc, temp2, zksi, xksi, yksi, thrid )          &
!$OMP SHARED   (npart_loc, pic1_loc, pic2_loc, twopinfp, zreduce_flag,    &
!$OMP           sgrid, ns, nsel_ubulk, msdmp, turbo_adi, Phi_bspl, qsde,  &
!$OMP           Apar_bspl, zcurr_flag, species, msdqs, zcos2, zsin2,      &
!$OMP           dphigrid_inv, phigrid, k_offset, dsgrid_inv, chigrid,     &
!$OMP           dchigrid_inv, rho_OMP, b_equ, nequ_zm1,                   &
!$OMP           nequ_rm1, nequ_z, nequ_r, iphipr, iphipl, nphip_min,      &
!$OMP           rgedz, rgedr, rphi_map, phi_edge, gez_max, gez_min,       &
!$OMP           ger_max, ger_min, nphip, kplw, jclw, islw, smax0,         &
!$OMP           me_cart, nidbas, ds_profiles_inv, t_s, ubulk_s, n_s, elmag)

   DO ip = 1, npart_loc
      thrid = OMP_GET_THREAD_NUM() + 1
      rt     = pic1_loc(R_PIC,ip)
      zt     = pic1_loc(Z_PIC,ip)
      phit   = pic1_loc(PHI_PIC,ip)
      ...
      rho_OMP(i,jjc,kkc,thrid) = rho_OMP(i,jjc,kkc,thrid) + temp2*ws(j)
      ...
   END DO
!$OMP END PARALLEL DO
   ...
   DO ii = 1, numthrds
      rho(:,:,:) = rho(:,:,:) + rho_OMP(:,:,:,ii)
   ENDDO

   DEALLOCATE (rho_OMP)
```

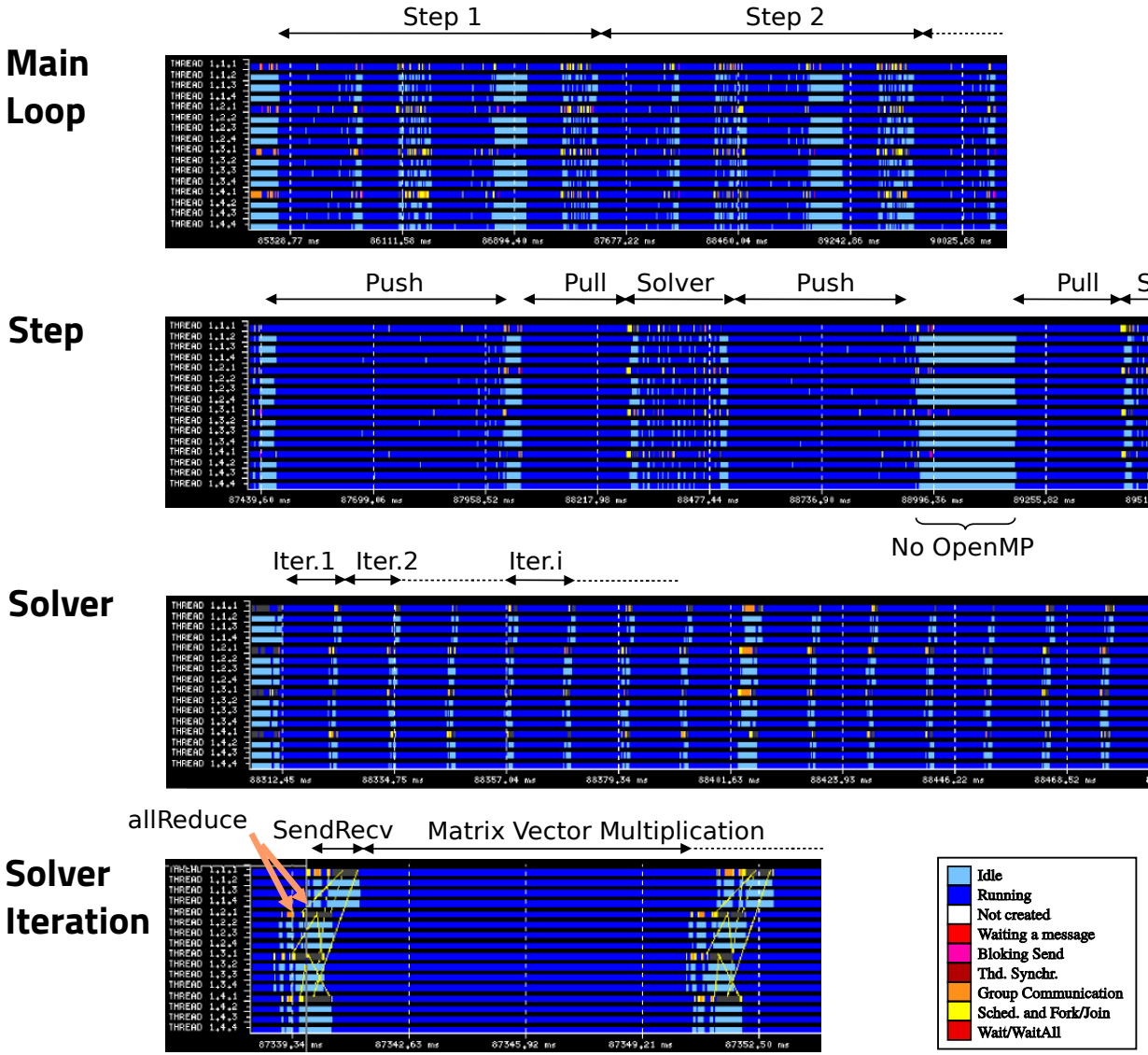
Thread Level Parallelism

- Solver Phase
  - Solve Linear Sparse Systems
  - PETSc issue → Not Thread-safe
  - Develop a thread-safe solver → JPCG and BJPCG

$$Ax = b$$

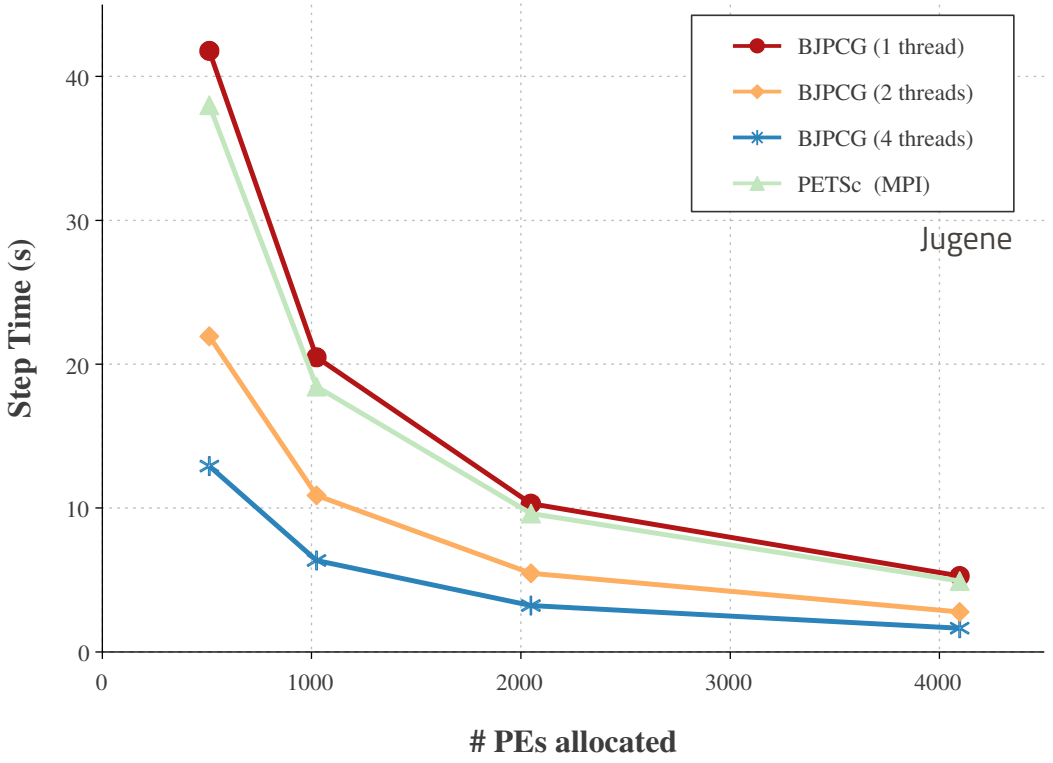
Thread Level Parallelism

- EUTERPE Hybrid version



Thread Level Parallelism

- EUTERPE Hybrid version

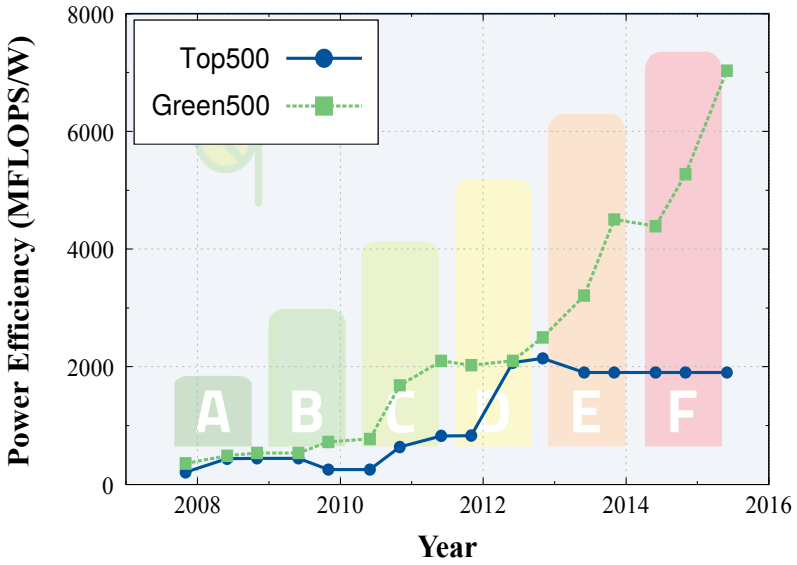


- 1,024 nodes
  - Original version can achieve 1,024 processors
  - Hybrid version can achieve 4,096 processors working with the same resources, so it improves the performance

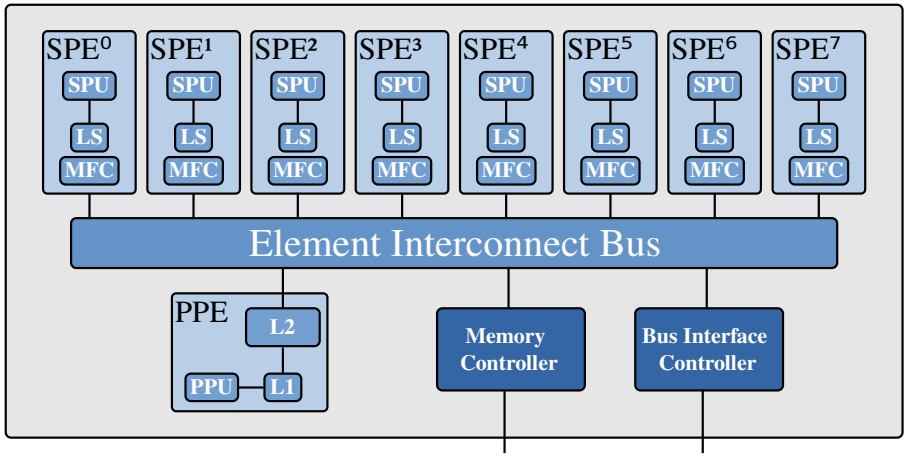
BJPCG:	128 blocks/process
Clone:	128 processes
Grid:	16x256x256
Particles:	10^9

Heterogeneous Parallelism

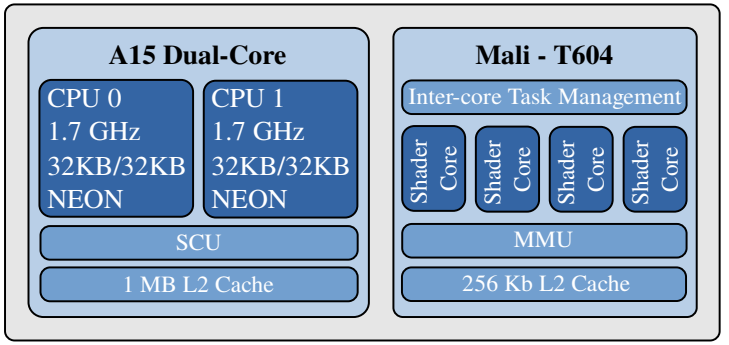
- Evolution



Cell (2009)



Samsung Exynos 5 Dual (2014)

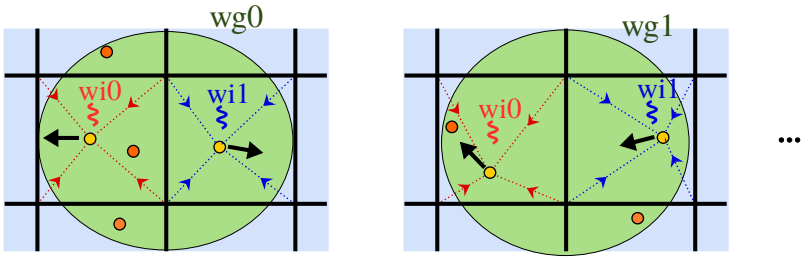


Heterogeneous Parallelism

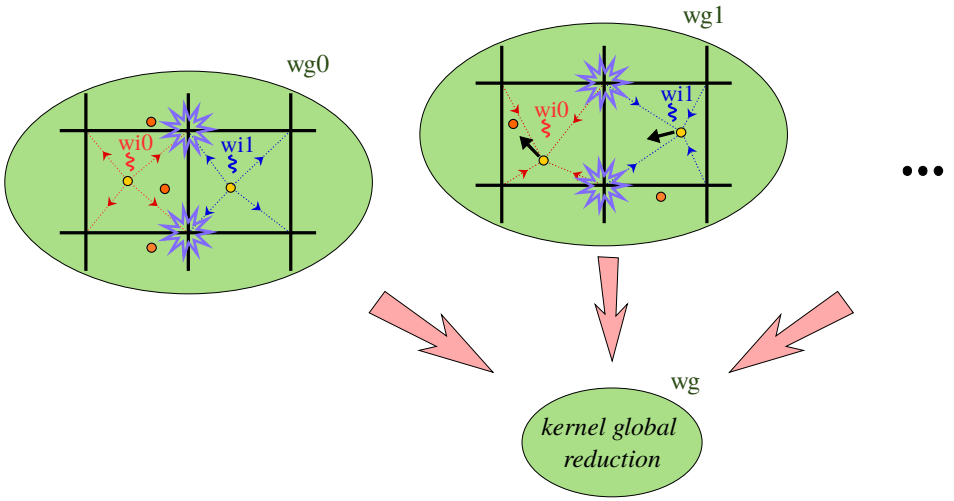
- Programming on Cell
  - Impressive peak performance → tedious programming process
    - Two different instruction sets (ISA)
    - DMA transfers → several alignment and size constraints
- ARM Mali GPU:
  - OpenCL (API) = improvement in the programming process
  - Unified memory system: local, private and global

Heterogeneous Parallelism

- Hybrid version (OpenMP + OpenCL)
  - OpenCL:
    - **Push**: similar OpenMP solution

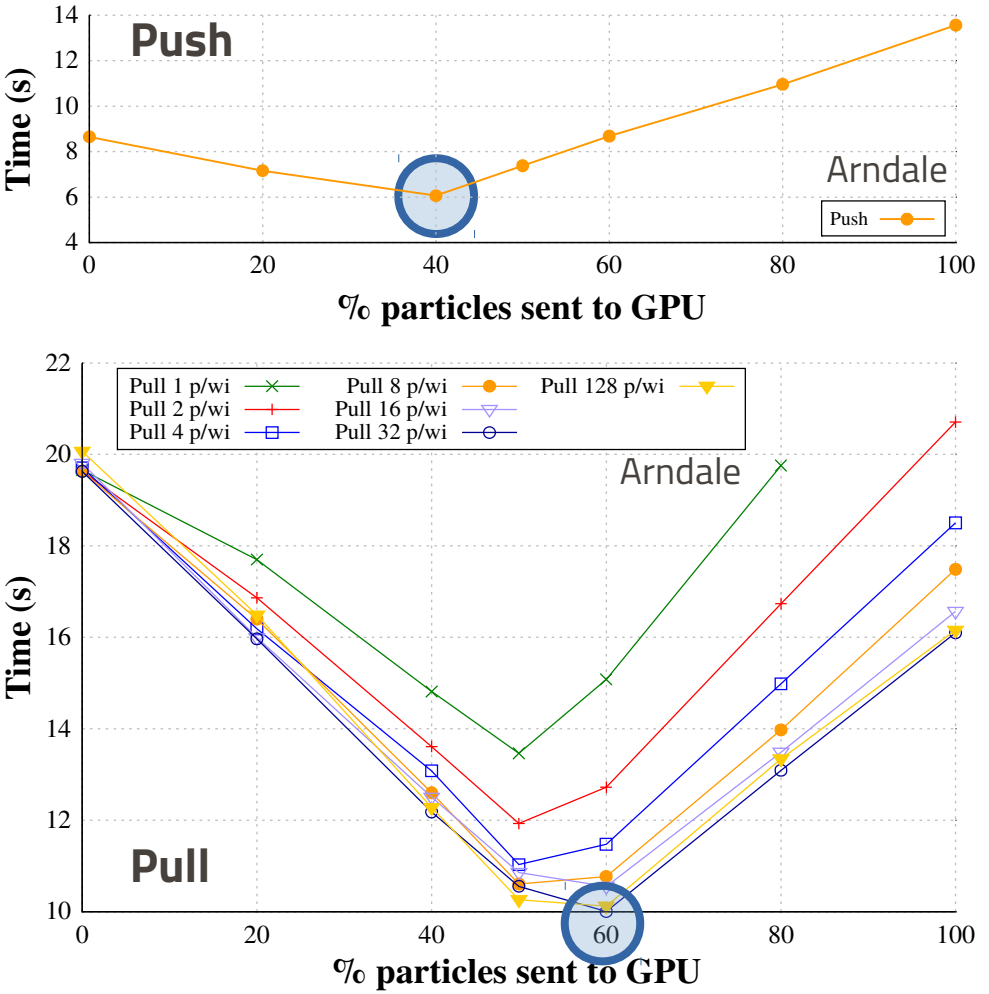


    - **Pull:** grid copy per work-group and atomics among work-items.



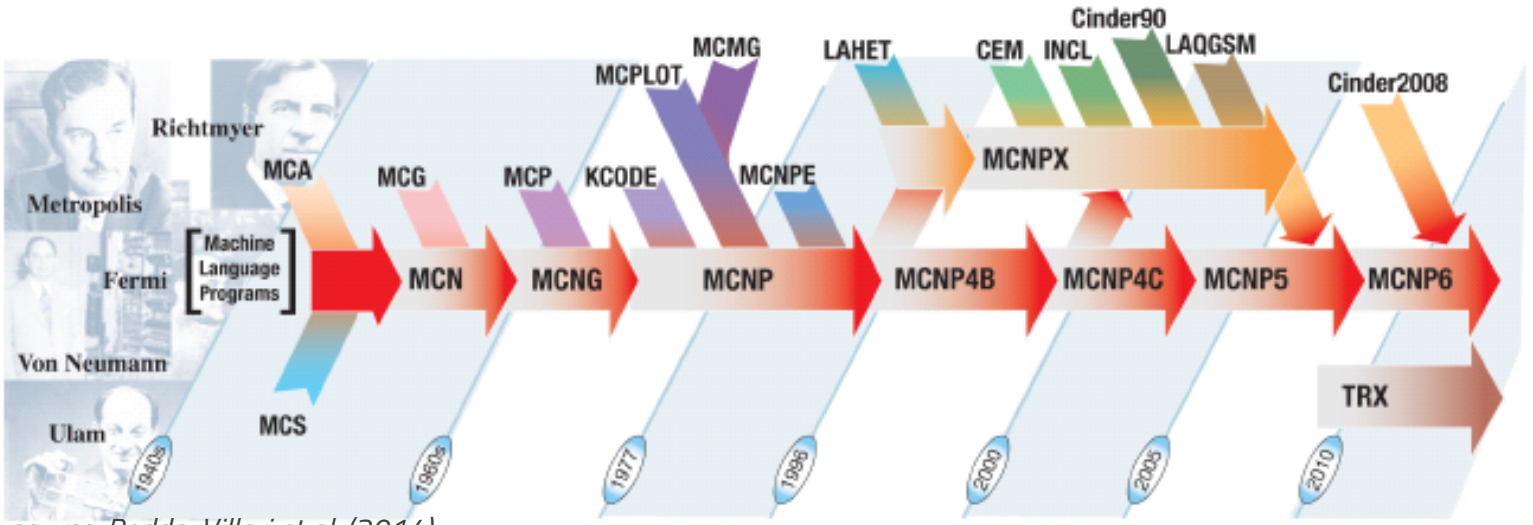
Heterogeneous Parallelism

- Hybrid version (OpenMP + OpenCL)
  - Hybrid version:
    - Static distribution of particles among devices (CPU and GPU)



Heterogeneous Parallelism

- But ...
  - Scientists are not in favor of porting production codes to new architectures:
    - It implies to re-validate the results
    - Codes are fruit of many collaborations



source: *Podda, Villari et al. (2014)*

MCNP6, fusion neutronics code developed from 1940s)

- A good solution could be a programming model that provides a certain level of abstraction over the hardware.

Heterogeneous Parallelism

- OmpSs (BSC)
  - Provides an abstraction that unifies SMP and heterogeneous programming in one model to reduce programmer effort
  - Taskification consists to reorganize some code to create taks (*groups of particles*).
- Push Phase

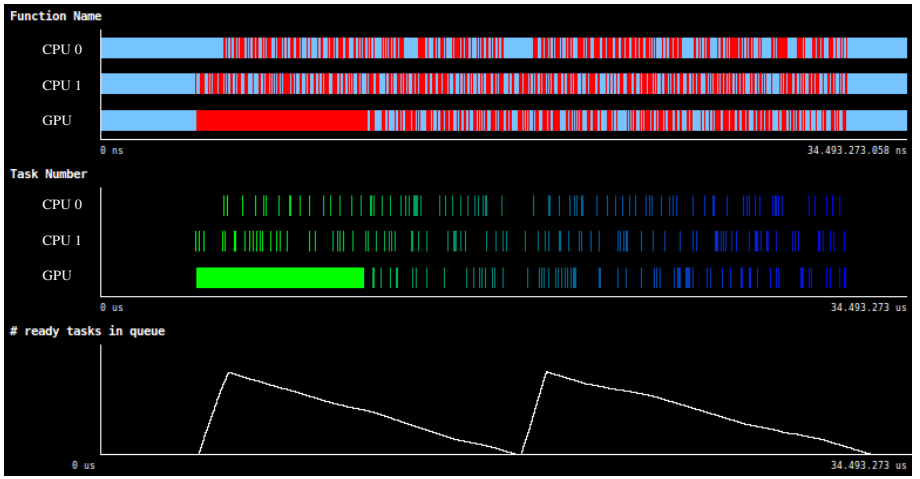
```
INTERFACE
   !$OMP copy_inout  (work1_loc(1:MAX_WORK, 1:(sup-inf+1)))    &
   !$OMP copy_in (pic1_loc, pic2_loc, msdqs, Phi_bspl,         &
   !$OMP          E_s_bspl, E_chi_bspl, E_phi_bspl, qsdms,     &
   !$OMP          msdmp, b_equ,sgrid, chigrid, phigrid,        &
   !$OMP          zcos2, zsin2, phieq, t_s, nsn_s, tst_s, n_s)

   !$OMP task  label(push_opencl)
   SUBROUTINE kernel_push (pic1_loc, pic2_loc, work1_loc,      &
   ...

   !$OMP target device(smp) implements (kernel_push)           &
   !$OMP copy_inout  (work1_loc(1:MAX_WORK, 1:(sup-inf+1)))    &
   !$OMP copy_in (pic1_loc, pic2_loc, msdqs, Phi_bspl,         &
   !$OMP          E_s_bspl, E_chi_bspl, E_phi_bspl, qsdms,     &
   !$OMP          msdmp, b_equ, sgrid, chigrid, phigrid,       &
   !$OMP          zcos2, zsin2, phieq, t_s, nsn_s, tst_s, n_s)

   !$OMP task  label(push_smp)
   SUBROUTINE kernel_push_smp (pic1_loc, pic2_loc, work1_loc,  &
   ...
END INTERFACE
```

```
CALL kernel_push (pic1_loc, pic2_loc, work1_loc(1,ipe),        &
                  species, dtloc, msdqs, qsdms, msdmp, ...
```



- Conclusion

Kernel	Performance - Best time (s)		Programmability - Productivity	
	OpenMP+OpenCL	OmpSs	OpenCL calls	OmpSs Directives
Push	6.02	6.92	161	12
Pull	10.31	10.83	167	18

- It is feasible to port a production PIC code to a heterogeneous platform
- OmpSs version is a bit slower but simpler → productivity ↑

Outline

Introduction to Plasma Physics

Supercomputing for Fusion Energy Applications

Particle-in-Cell Codes

- Fusion Group

Fusion Group

- Members
  - Mervi Mantsinen
  - Felipe Nathan de Oliveira
  - Shimpei Futatani
  - Dani Gallart
  - Albert Gutiérrez
  - Allah Rakah
  - Carles Riera
  - Xavier Sáez
- Research
  - Optimization of fusion applications
  - Understanding and control of ELM physics
  - Modelling of Ion Cyclotron Resonance Frequency Heating (ICRF)
  - Modelling DEMO reactor
  - Magnetohidrodynamics (MHD) and instabilities
  - Fusion neutronics

Fusion Group

- Collaborations

- More information
  - Blog: fusion.bsc.es (under construction)
  - Web: www.bsc.es
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Thanks for your attention!